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**Prediction of Advanced Nitramine Propellant  
Burning Rates With the CYCLOPS Code**

**by Martin S. Miller and William R. Anderson**

ARL-MR-552

March 2003

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# **Army Research Laboratory**

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**Weapons and Materials Research Directorate, ARL**

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## 1. Introduction

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In addition to the scientific and technological challenges, fielding a new propellant is accompanied by a well-documented set of financial, organizational, and environmental burdens (Miller et al. 2000). To be successful, a new propellant formulation must be characterized by and satisfy a long, hierarchical series of measurements and tests. Candidate formulations that look promising at some stage in development may fail later tests, and then new formulations must start the battery of sequential and parallel tests all over again. The early “inner-loop” measurements will therefore be performed a very large number of times and result in large accumulated costs and waste streams. Any theoretical assistance in obviating the need for these measurements will therefore pay large dividends. One of the inner-loop propellant properties that currently must be measured is the linear burning rate. This property has a direct bearing on the rate of energy release in a gun or rocket and is a critical input to interior-ballistic design codes. Being a nonequilibrium property, the burning rate is a very complex function of physical and reactive processes that, despite decades of intensive research, are not thoroughly understood. Thus, only modest progress has been made toward the goal of predicting the burning rates of energetic materials. Though considerable sophistication has been achieved in describing gas-phase transport and chemical reactions, the knowledge of the mechanisms and reactions taking place in the condensed phase of the energetic material is scant and highly speculative.

Into this stalemated situation we introduced a new semiempirical approach for the burning-rate calculations to circumvent the uncertainties of the condensed phase and capitalize on the growing body of knowledge of the gas-phase reactions and reaction mechanisms (Miller and Anderson 2000). The new model made use of the important, previously discovered fact that the quantitative relationship between the burning rate and the burning surface temperature (known as the pyrolysis law) is approximately independent of the type of energetic material in its functional form and even approximately independent of ingredient proportions for double-base propellants. The semiempirical model has recently been successfully extended to treat multiingredient nitrate-ester propellants (i.e., those containing various proportions of nitroglycerine, diethylene glycol dinitrate [DEGDN], and nitrocellulose of varying nitration levels), enabling credible predictions of the burning rate for a number of double-base formulations (Miller and Anderson 2002). This multiingredient code was named CYCLOPS after the mythical race of creatures that forged thunderbolts for Zeus. We show in this report that the universal character of the pyrolysis law (with different parameters) is also approximately valid for propellants using cyclotrimethyletrinitramine (RDX) and cyclotetramethylenetetranitramine (HMX) in a wide range of polymeric binders. Early indications are that the same is true of hexanitrohexaazaisowurtzitane (CL20) propellants, although the parameters of the pyrolysis law are very different than for the RDX/HMX nitramine propellants, and only one binder has currently

been characterized. Having established this, it made sense to apply the semiempirical burning-rate model to these two types of nitramine propellants. The encouraging first results of these efforts are presented in this report.

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## 2. Pyrolysis Laws

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Professor Anatoli Zenin at the Semenov Institute of Chemical Physics in Moscow has distinguished himself for more than 40 years as the consummate practitioner of experiments in which micron-sized thermocouples are embedded in propellant specimens and then burned to produce temperature profiles of the reaction zones during combustion. Zenin perfected this technique over decades mostly with double-base propellants of widely varying formulations. His work showed the universal character of the pyrolysis law (equation 1) for this important class of propellants (e.g., Zenin 1995). The quality of this idealization is shown in Figure 1. The relationship holds for proportions of nitroglycerine from 0% to 50% and nitrocellulose nitration levels from 11% to 13% (Zenin 1999).

$$m = m_0 e^{-\frac{E_s}{RT_s}} \quad (1)$$

For the last few years, the U.S. Army Research Office/European Research Office has been funding Professor Zenin to make microthermocouple measurements on propellants composed of RDX and HMX and a variety of nonenergetic and energetic polymers (Zenin 1998, 2000). Most recently, the professor has begun studying CL20 in different binders. (These results are also shown in Figure 1.) It can be seen that the class of propellants with RDX or HMX in a variety of binders exhibits the same universal character, although with different parameters and with somewhat greater scatter about the fit. We have obtained a pyrolysis law using all of the RDX and HMX data with binders by least squares analysis; this law is designated NTRB (nitramine/binder). To determine the sensitivity of the computed burning rates to uncertainties in the pyrolysis law, we also obtained a pyrolysis law using only the RDX/bisazidomethylene oxetane-azidomethylenemethyl oxetane (BAMO-AMMO) data; this is termed RDXBAZ (RDX-BAMO-AMMO-Zenin). At this writing, Zenin has completed work (Zenin 2002) on only one CL20/binder combination—that binder is PUNE, a polyurethane rubber plasticized by a mixture of two nitroesters, dinitratdieteneglycole and dinitrattributylenglicole. The pyrolysis law derived from this data is designated CL20B. Other binders are currently being investigated. We will presume in this work that CL20B will work for other binders as well, though this remains to be proved. The pyrolysis law parameters for these cases are given in Table 1.

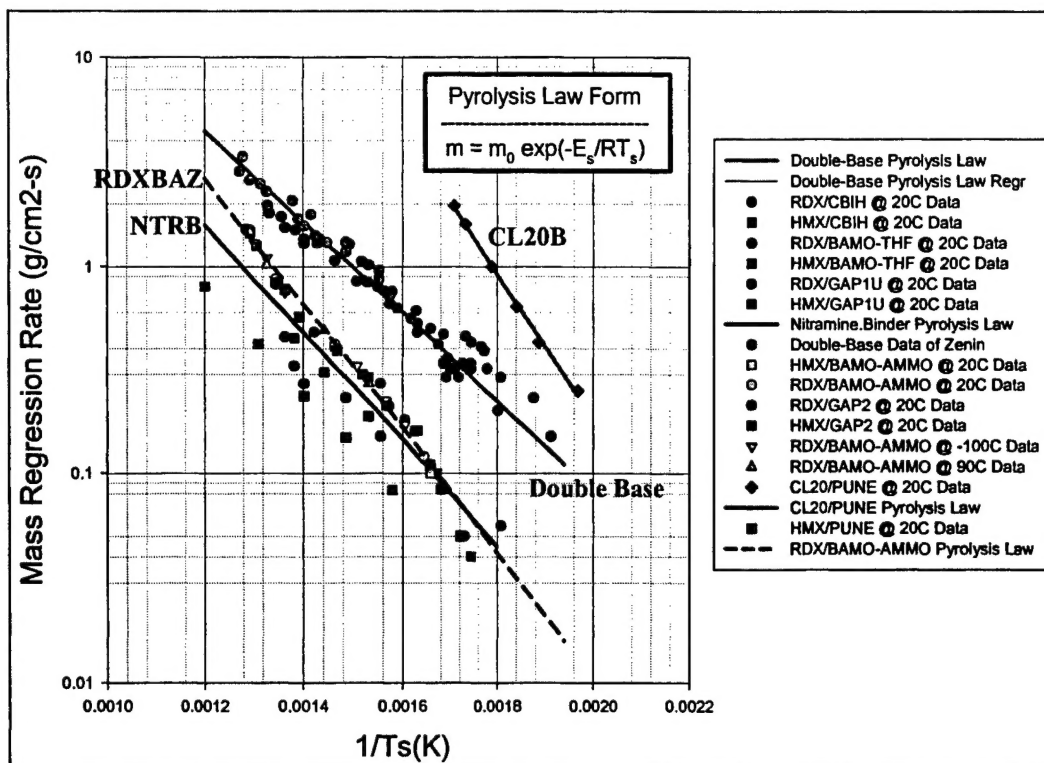


Figure 1. Pyrolysis law experimental data (symbols) and fits to equation 1 for different propellant types.

Table 1. Pyrolysis law parameters.

Pyrolysis Law	$m_0$ (g/cm <sup>2</sup> -s)	$E_s$ (cal/mole)
NTRB	2004	11827
RDXBAZ	10470	13720
CL20B	1868000	16032

### 3. Condensed-Phase Decomposition Products

In addition to the pyrolysis law, the semiempirical theory requires an estimate of the condensed-phase decomposition products for each of the ingredients making up the propellant. Since RDX has a high vapor pressure and is believed mainly to simply vaporize during combustion as a monopropellant (Miller and Anderson 2000), we chose to assume that RDX vapor is the product of condensed-phase RDX leaving the surface. This assumption proved successful in the previous application of the present model to the combustion of neat RDX (Miller and Anderson 2000).



BAMO and AMMO are both energetic polymers being considered as binders for advanced nitramine propellants. Their structure is represented schematically in Figures 2 and 3.

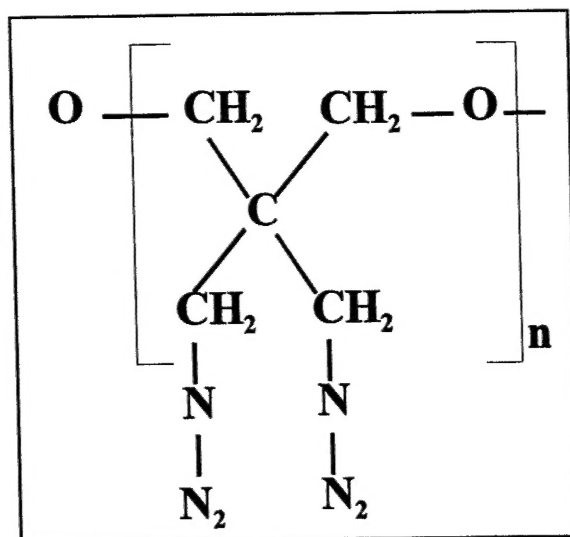


Figure 2. Schematic structure of BAMO.

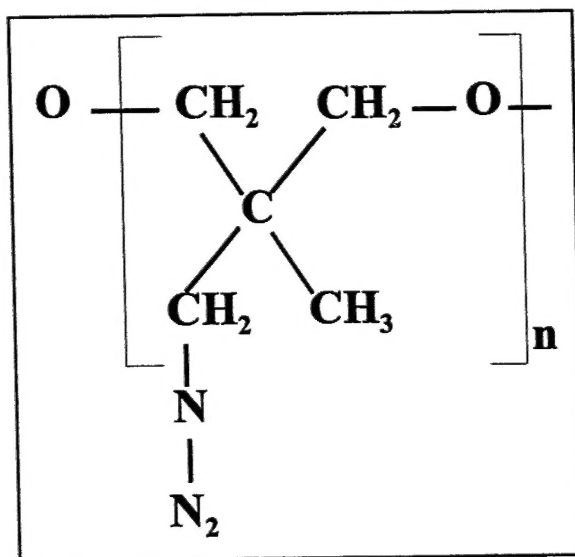
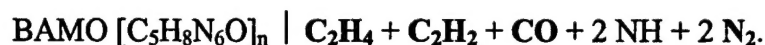


Figure 3. Schematic structure of AMMO.

A number of different sets of products for BAMO and AMMO were tried, roughly consistent with published measurements of their decomposition products. Experiments rarely give a neat set of products leading to a chemically balanced equation. In our calculations, we constrain our selected product sets to be chemically balanced and do the best we can to include those products seen experimentally. Although there are a great many possible decomposition product sets that lead equally well to chemical balance, we most often find that different product sets lead to very different burning rates so that a particular set usually recommends itself. For BAMO and AMMO, the best product sets that we found are as follows:



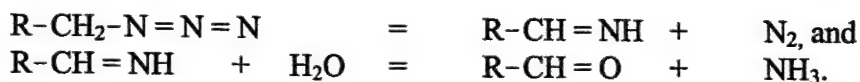
The species in bold-face type have been identified experimentally as thermal decomposition products of AMMO and BAMO by Chen and Brill (1991), Brill and Brush (1992), Roos and Brill (2000), and Lee et al. (1998, 1999).

The astute chemist will no doubt note that it seems unlikely that the ejection of radicals (e.g., NH in the previous product lists) is what is actually taking place. This event would require the breaking of a strong chemical bond(s) in a species close to the propellant melt layer at a temperature of only about 400–600 K. At so cool a temperature, such a high-energy bond breaking step(s) would likely be quite slow. In addition, unless the radical is produced in the monolayer at the surface, it is likely to collide with other species on its way towards the condensed-gas phase boundary. Because of the highly reactive nature of radicals, the identity of the radical is likely to change on its way to the surface. However, while we make every attempt to favor those decomposition-product sets that are consistent with experiments, we do not limit ourselves only to those species which are observed or which even seem the most likely. The ultimate arbiter of appropriateness is agreement of the model predictions of burning rates with measured ones. There are two reasons for this pragmatic approach. The first is that experiments rarely allow a complete chemically balanced set of products to be deduced. Second, experiments may not be able to measure some reactive radicals because of unavoidable secondary reactions; with monolithic adherence to the inclusion of only measured species, one might easily miss some essential high-heat reactions.

Thus, if it is necessary to assume a high concentration of radicals is released at the propellant surface to get good agreement with experiment for certain ingredients, this is what is done. It is then presumed that the results will yield accurate predictions for propellants that are mixtures of the various ingredients modeled.

An important point concerning the BAMO and AMMO product sets is that both BAMO and AMMO contain azide groupings,  $R - N = N = N$  (see Figures 2 and 3). Although it is difficult to see how the BAMO-AMMO units might directly produce  $NH$ , they are known to produce  $NH_3$  in pyrolysis experiments (Chen and Brill 1991; Brill and Brush 1992; Roos and Brill 2000; Lee et al. 1998, 1999). Note that if  $NH$  actually is ejected into the gas phase from the surface, it would not have been detected in those experiments because the radical is so reactive that it would be converted to stable species prior to detection (e.g.,  $NH_3$  as observed). As  $NH_3$  reacts in the gas phase, it produces  $NH_x$  species,  $x = 0 - 2$ , including  $NH$ . Conceivably, if this happens in the condensed phase near surface region,  $NH$  might actually be ejected, though, as we have stated, this seems unlikely. However, the  $NH_x$  chemistry brought into play by assuming  $NH$  is one of the surface products is undoubtedly similar to that in the actual propellants, where the pyrolysis experiments strongly suggest that  $NH_x$  species must have been produced. Our main purpose in selecting surface product sets is to be able to reproduce observed experimental results for individual ingredients and then use those same assumptions for propellant mixtures. Obviously, by use of the surface product sets for the individual ingredients as calculated from the proportions of the ingredients, we assume that the ingredients break down in the condensed phase without any chemical interaction of ingredients or the intermediate species within the condensed phases. Our empirical approach is only justified insofar as the experimental data for the mixtures is then reproduced. As shown previously for nitrate ester propellants, and herein for nitramine propellants, the approach works well. It should be noted that we did try a product set with  $NH_3$ , but it led to predicted burning rates which had the wrong pressure dependence.

There have been extensive studies on methyl and ethyl azide decomposition. These suggest that  $NH_3$  can be produced by the following reaction sequence:



Regarding the first of these, it has been shown in experimental studies that  $R-CH=NH + N_2$  is the primary reaction pathway for methyl and ethyl azides under thermal conditions (see O'Dell and Darwent 1970; Bock and Dammel; 1988, and references therein). A number of theoretical studies have also been performed on methyl and ethyl azides (see Nguyen et al. 1996; Arenas et al. 2000, 2001; and references therein). There has been some controversy regarding whether the first step takes place primarily via (1) an elementary reaction with transition state involving concerted elimination of  $N_2$  and motion of one of the H atoms across the C-N bond to produce the imine product,  $CH_2=NH$ , in the case of methyl azide or (2)  $N_2$  is first eliminated, leading, in the case of methyl azide, to  $CH_3N$ . The  $CH_3N$  can then undergo a 1,2 hydrogen shift, resulting in  $CH_2=NH$ . And either  $CH_3N$  or  $CH_2=NH$  could eliminate  $H_2$ , leading to  $HCN$ . In the studies where it is concluded that  $N_2$  is first eliminated, there has also been a great deal of interest regarding whether the reaction takes place primarily on a singlet or triplet potential energy surface. The most recent work suggests that the two may be equally important. However, all of the studies support the notion

that  $R-CH = NH + N_2$  could be the most important overall pathway. The second of the reactions just shown may not be an elementary step as written, especially when one considers that it involves considerable rearrangement and that in the case of propellants, it may be taking place in a liquid melt layer.

A new energetic material with high-energy density that is being considered as a crystalline filler for advanced nitramine propellants is CL20, depicted schematically in Figure 4.

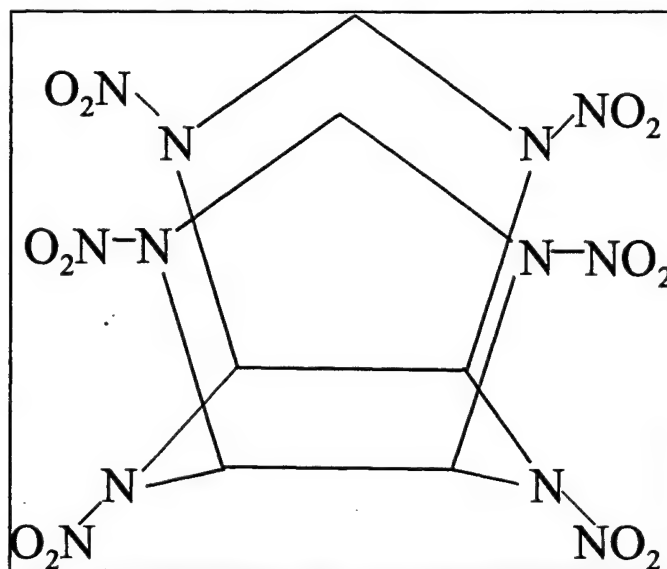
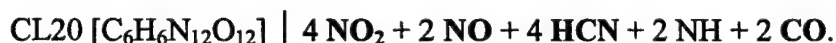


Figure 4. Schematic structure of CL20.

The best set of decomposition products found for CL20 is as follows:



Again, in boldface type are the species seen experimentally in thermal decomposition experiments by Chen and Brill (1991).

## 4. Reaction Mechanism

The gas-phase chemical reaction mechanism, comprising a set of 80 species and 550 reversible elementary reversible reactions, their rate coefficients, and thermodynamic functions, was used in this work. The starting point for developing this mechanism was the much smaller mechanism used by Liao (1997) and others, consisting of 45 species and 232 reversible elementary reactions. The new mechanism is given in the Appendix in the form provided by the CHEMKIN code as an output file. The extensive modifications to this older mechanism required estimation of many reaction-rate coefficients using the Quantum-Rice-Ramsperger-Kassel theory and will be detailed in a future report.

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## 5. Results

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Some burning-rate data exist for BAMO and AMMO but the rate is slow and we were unable to achieve convergence of the PREMIX code for this slow flame. We therefore went directly to the RDX/BAMO-AMMO mixture, assuming that RDX evaporated from the surface of the propellant as it did when neat. Figure 5 shows the results of the calculation for the mixture of RDX and BAMO-AMMO used by Zenin, with both the NTRB and RDXBAZ pyrolysis laws. It is clear that, at least in this case, no great error arises from using the more general NTRB law. This is important because it reinforces our assumption of "universality" for this family of propellants.

Our usual implementation of the method embodied in the CYCLOPS code is to first apply the model to neat ingredients and then to propellant mixtures. There is currently no data to obtain a pyrolysis law for neat CL20, so we were forced to deal directly with the CL20 propellant mixture with BAMO-AMMO as a binder. Fortunately, the results for RDX/BAMO-AMMO were encouraging enough to make an attempt worthwhile by using the successful product decomposition set found for BAMO-AMMO in the RDX-based propellant. Results of the burning-rate calculations for the CL20/BAMO-AMMO propellant are given in Figure 6. In view of the fact that the experimental data for both pyrolysis law and burning rates are preliminary in nature, the agreement between CYCLOPS and the experiment is excellent. The variance at the highest pressures is currently unexplained but could be due to faults in the reaction mechanism at that pressure or changes in the decomposition products with pressure, experimental error, or some combination of these factors.

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## 6. Flame Structure

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The gas-phase temperature profile under steady-state combustion conditions at a pressure of 10 atm and an initial temperature of 20 °C was measured by Zenin (2000) for the RDX/BAMO-AMMO propellant being considered here. This measure profile is compared with the predicted profile in Figure 7. It can be seen that the measured profile extends to a considerably larger distance from the surface than the predictions would suggest and exhibits a more pronounced dark zone than predicted. The predicted profile does, however, show an inflection at about the same temperature as the experimental one. The distance scale of the measured profile is very small, only about 1 mm. Given the finite response time of the thermocouple used in the measurement, it is possible that the differences seen in the figure arise because of experimental errors. On the other hand, it is possible that there is some inaccuracy in those reaction rate coefficients associated with the onset of the visible flame while not affecting those reactions

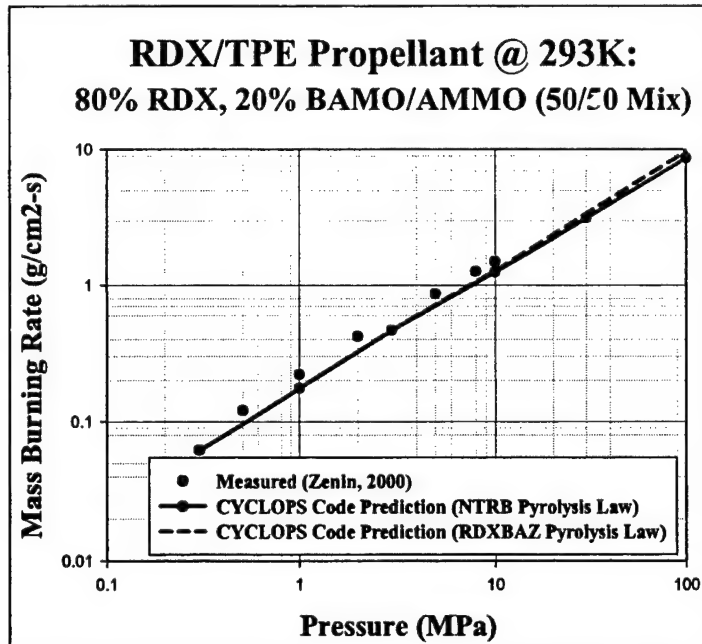


Figure 5. Comparison of experimental and CYCLOPS-predicted burning rates as a function of pressure for a propellant consisting of 80% RDX in 20% binder of BAMO and AMMO (50/50 mix). The solid theoretical curve employed the NTRB pyrolysis law and the dashed curve the RDXBAZ pyrolysis law.

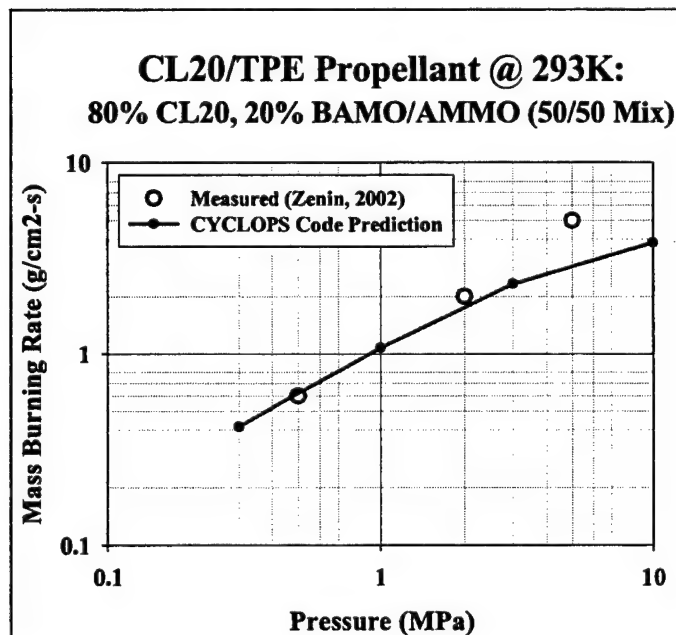


Figure 6. Computed burning rate of an advanced nitramine propellant compared with measured rates.

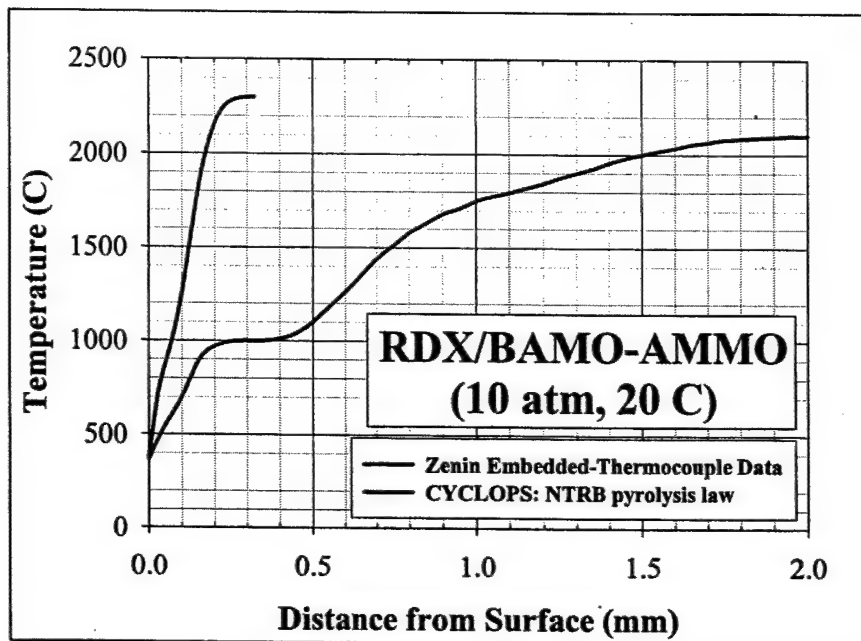


Figure 7. Gas-phase reaction-zone temperature profile as measured by Zenin (2000) (curve that extends to 2 mm) and as computed by the CYCLOPS code.

contributing to the burning rate itself. This could explain the excellent agreement between the model and the experiment for burning rate and discrepancy in flame structure. The choice of condensed-phase reaction products could also not be optimum. Calculations of the flame structure using the RDXBAZ pyrolysis law show no difference from the NTRB pyrolysis law results shown. Future work may resolve this issue.

## 7. Conclusions

Due to a lack of understanding of the condensed-phase and surface processes, a first-principles calculation of the burning rates of energetic materials and propellants is impossible at the present time. In our judgment, this situation is likely to persist for many years to come, yet theoretical guidance in the formulation of advance propellants is urgently needed to meet current financial and environmental constraints. We have developed a practical semiempirical model for predicting the burning rates of multiingredient propellants, and it has previously been shown to give credible results for nitrate-ester propellants. In this report, we have applied the model to advanced propellant formulations involving RDX, CL20, and the BAMO/AMMO energetic binder. Results are not perfect but, given the enormous complexities of the problem (80 species and 550 reversible reactions), they are surprisingly good. In its present form, this model could prove useful in optimizing propellant-formulation variables such as ingredient proportions and possibly also in predicting the effect of combustion modifiers on the burning rate and flame

structure, as was briefly explored for a few small-molecule additives in previous work (Miller and Anderson 2000). To the extent that a one-dimensional model is valid, our approach depends for its predictive accuracy on the reliability of its three principal inputs—a gas-phase reaction mechanism, an empirical pyrolysis law linking the mass burning rate with surface temperature, and a set of condensed-phase decomposition products. With accurate inputs, one can expect accurate predictions of burning rate. Since our knowledge of the elementary reactions that may be important and their rate coefficients is constantly improving and new measurements of thermal decomposition of propellant ingredients are continually becoming available, one can expect that the burning rates predicted by CYCLOPS will likewise continually improve. However, it is worth emphasizing that even semiquantitative predictions may prove valuable to systematic formulation studies, the search for useful chemical additives, and guidance in the setting of specifications for ingredient purity and proportion tolerances.

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## **Appendix . Gas-Phase Reaction Mechanism**

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This appendix appears in its original form, without editorial change.

CHEMKIN INTERPRETER OUTPUT: CHEMKIN-II Version 3.6 Apr. 1994  
DOUBLE PRECISION

ELEMENTS CONSIDERED	ATOMIC WEIGHT
1. AR	39.9480
2. C	12.0112
3. H	1.00797
4. N	14.0067
5. O	15.9994

SPECIES CONSIDERED	C P H H A A R		S G MOLECULAR		TEMPERATURE		ELEMENT COUNT				
	E E WEIGHT		LOW		HIGH		AR	C	H	N	O
1. AR	G 0	39.94800	300.0	5000.0	1	0	0	0	0	0	0
2. H2	G 0	2.01594	300.0	5000.0	0	0	2	0	0	0	0
3. O2	G 0	31.99880	300.0	5000.0	0	0	0	0	0	2	0
4. H2O	G 0	18.01534	300.0	5000.0	0	0	2	0	1	0	0
5. O	G 0	15.99940	300.0	5000.0	0	0	0	0	0	1	0
6. H	G 0	1.00797	300.0	5000.0	0	0	1	0	0	0	0
7. OH	G 0	17.00737	300.0	5000.0	0	0	1	0	1	0	0
8. HO2	G 0	33.00677	200.0	6000.0	0	0	1	0	2	0	0
9. H2O2	G 0	34.01474	300.0	5000.0	0	0	2	0	2	0	0
10. CH2O	G 0	30.02649	200.0	3500.0	0	1	2	0	1	0	0
11. HCO	G 0	29.01852	200.0	6000.0	0	1	1	0	1	0	0
12. CO	G 0	28.01055	300.0	5000.0	0	1	0	0	1	0	0
13. CO2	G 0	44.00995	300.0	5000.0	0	1	0	0	2	0	0
14. N	G 0	14.00670	200.0	6000.0	0	0	0	1	0	0	0
15. N2	G 0	28.01340	300.0	5000.0	0	0	0	2	0	0	0
16. NO	G 0	30.00610	200.0	6000.0	0	0	0	1	1	0	0
17. NO2	G 0	46.00550	200.0	6000.0	0	0	0	1	2	0	0
18. NH	G 0	15.01467	200.0	6000.0	0	0	1	1	0	0	0
19. NH2	G 0	16.02264	200.0	6000.0	0	0	2	1	0	0	0
20. NH3	G 0	17.03061	200.0	6000.0	0	0	3	1	0	0	0
21. NNH	G 0	29.02137	300.0	5000.0	0	0	1	2	0	0	0
22. HNO	G 0	31.01407	200.0	6000.0	0	0	1	1	1	0	0
23. HONO	G 0	47.01347	300.0	5000.0	0	0	1	1	2	0	0
24. HCN	G 0	27.02582	200.0	6000.0	0	1	1	1	0	0	0
25. HNC	G 0	27.02582	300.0	5000.0	0	1	1	1	0	0	0
26. N2O	G 0	44.01280	200.0	6000.0	0	0	0	2	1	0	0
27. CN	G 0	26.01785	200.0	6000.0	0	1	0	1	0	0	0
28. C2N2	G 0	52.03570	300.0	5000.0	0	2	0	2	0	0	0
29. NCN	G 0	40.02455	300.0	4000.0	0	1	0	2	0	0	0
30. NCO	G 0	42.01725	200.0	6000.0	0	1	0	1	1	0	0
31. CNO	G 0	42.01725	300.0	4000.0	0	1	0	1	1	0	0
32. HNCO	G 0	43.02522	200.0	6000.0	0	1	1	1	1	0	0
33. HOCN	G 0	43.02522	300.0	4000.0	0	1	1	1	1	0	0
34. HCNO	G 0	43.02522	300.0	5000.0	0	1	1	1	1	0	0
35. NO3	G 0	62.00490	300.0	5000.0	0	0	0	1	3	0	0
36. HNO3	G 0	63.01287	300.0	5000.0	0	0	1	1	3	0	0
37. H2CN	G 0	28.03379	300.0	4000.0	0	1	2	1	0	0	0
38. H2CNH	G 0	29.04176	300.0	4000.0	0	1	3	1	0	0	0
39. H2CNO	G 0	44.03319	300.0	4000.0	0	1	2	1	1	0	0
40. H2CNNO	G 0	58.03989	300.0	4000.0	0	1	2	2	1	0	0
41. H2CNNO2	G 0	74.03929	300.0	4000.0	0	1	2	2	2	0	0
42. H2COHNO2	G 0	91.04666	300.0	4000.0	0	1	3	2	3	0	0
43. RDX	G 0	222.11787	300.0	4000.0	0	3	6	6	6	0	0
44. RDXR	G 0	176.11237	300.0	4000.0	0	3	6	5	4	0	0
45. RDXRO	G 0	176.11237	300.0	4000.0	0	3	6	5	4	0	0
46. HNNO	G 0	45.02077	300.0	5000.0	0	0	1	2	1	0	0
47. N2H2	G 0	30.02934	200.0	6000.0	0	0	2	2	0	0	0
48. N2H3	G 0	31.03731	300.0	5000.0	0	0	3	2	0	0	0
49. N2H4	G 0	32.04528	300.0	5000.0	0	0	4	2	0	0	0

50. H2NN	G 0	30.02934	300.0	5000.0	0	0	2	2	0
51. NH2NO	G 0	46.02874	300.0	5000.0	0	0	2	2	1
52. NH2O	G 0	32.02204	300.0	5000.0	0	0	2	1	1
53. NH2OH	G 0	33.03001	200.0	6000.0	0	0	3	1	1
54. HNOH	G 0	32.02204	300.0	5000.0	0	0	2	1	1
55. HNNNH2	G 0	45.04401	300.0	5000.0	0	0	3	3	0
56. H2NNHO	G 0	47.03671	300.0	5000.0	0	0	3	2	1
57. CH3	G 0	15.03506	300.0	5000.0	0	1	3	0	0
58. CH4	G 0	16.04303	300.0	5000.0	0	1	4	0	0
59. HONHO	G 0	48.02144	300.0	5000.0	0	0	2	1	2
60. HNOO	G 0	47.01347	300.0	5000.0	0	0	1	1	2
61. HNO2	G 0	47.01347	300.0	5000.0	0	0	1	1	2
62. HON	G 0	31.01407	300.0	5000.0	0	0	1	1	1
63. HNNHO	G 0	46.02874	300.0	5000.0	0	0	2	2	1
64. HOONO	G 0	63.01287	300.0	5000.0	0	0	1	1	3
65. CH	G 0	13.01912	300.0	5000.0	0	1	1	0	0
66. C	G 0	12.01115	300.0	5000.0	0	1	0	0	0
67. CH2	G 0	14.02709	250.0	4000.0	0	1	2	0	0
68. CH2 (S)	G 0	14.02709	300.0	4000.0	0	1	2	0	0
69. CH2OH	G 0	31.03446	250.0	4000.0	0	1	3	0	1
70. CH3O	G 0	31.03446	300.0	3000.0	0	1	3	0	1
71. CH3OH	G 0	32.04243	300.0	5000.0	0	1	4	0	1
72. C2H	G 0	25.03027	300.0	4000.0	0	2	1	0	0
73. HCCO	G 0	41.02967	300.0	4000.0	0	2	1	0	1
74. C2H2	G 0	26.03824	300.0	5000.0	0	2	2	0	0
75. C2H3	G 0	27.04621	300.0	5000.0	0	2	3	0	0
76. CH2CO	G 0	42.03764	300.0	5000.0	0	2	2	0	1
77. C2H4	G 0	28.05418	300.0	5000.0	0	2	4	0	0
78. C2H5	G 0	29.06215	300.0	5000.0	0	2	5	0	0
79. C2H6	G 0	30.07012	300.0	4000.0	0	2	6	0	0
80. HCCOH	G 0	42.03764	300.0	4000.0	0	2	2	0	1

REACTIONS CONSIDERED		(k = A T**b exp(-E/RT))		
		A	b	E
1. H2+M=H+H+M		4.570E+19	-1.40	104000.0
H2	Enhanced by	2.500E+00		
H2O	Enhanced by	1.200E+01		
CO	Enhanced by	1.900E+00		
CO2	Enhanced by	3.800E+00		
N2O	Enhanced by	5.000E+00		
NH3	Enhanced by	5.000E+00		
2. O+H2=H+OH		5.060E+04	2.67	6290.0
3. O+O+M=O2+M		6.170E+15	-0.50	0.0
H2	Enhanced by	2.500E+00		
H2O	Enhanced by	1.200E+01		
CO	Enhanced by	1.900E+00		
CO2	Enhanced by	3.800E+00		
N2O	Enhanced by	5.000E+00		
4. H+O2=O+OH		1.940E+14	0.00	16440.0
5. H+O2 (+M)=HO2 (+M)		4.520E+13	0.00	0.0
Low pressure limit:	0.67000E+20	-0.14200E+01	0.00000E+00	
TROE centering:	0.10000E+01	0.10000E-89	0.10000E+91	
H2	Enhanced by	2.500E+00		
H2O	Enhanced by	1.200E+01		
CO	Enhanced by	1.900E+00		
CO2	Enhanced by	3.800E+00		
N2O	Enhanced by	5.000E+00		
NH3	Enhanced by	5.000E+00		
6. H+O+M=OH+M		4.720E+18	-1.00	0.0
H2	Enhanced by	2.500E+00		
H2O	Enhanced by	1.200E+01		
CO	Enhanced by	1.900E+00		
CO2	Enhanced by	3.800E+00		
N2O	Enhanced by	5.000E+00		
7. OH+H2=H2O+H		2.160E+08	1.51	3430.0
8. OH+OH=H2O+O		3.570E+04	2.40	2112.0
9. OH+H+M=H2O+M		2.210E+22	-2.00	0.0

H2	Enhanced by	2.500E+00		
H2O	Enhanced by	1.200E+01		
CO	Enhanced by	1.900E+00		
CO2	Enhanced by	3.800E+00		
N2O	Enhanced by	5.000E+00		
10. HO2+O=O2+OH		1.750E+13	0.00	-397.0
11. H+HO2=H2+O2		4.280E+13	0.00	1411.0
12. H+HO2=2OH		1.690E+14	0.00	874.0
13. H+HO2=O+H2O		3.010E+13	0.00	1721.0
14. HO2+OH=H2O+O2		1.900E+16	-1.00	0.0
15. HO2+HO2=H2O2+O2		4.200E+14	0.00	11980.0
Declared duplicate reaction...				
16. HO2+HO2=H2O2+O2		1.300E+11	0.00	-1629.0
Declared duplicate reaction...				
17. H2O2(+M)=OH+OH(+M)		2.950E+14	0.00	48460.0
Low pressure limit:	0.12000E+18	0.00000E+00	0.45500E+05	
TROE centering:	0.50000E+00	0.10000E-89	0.10000E+91	
N2O	Enhanced by	5.000E+00		
H2O	Enhanced by	1.200E+01		
N2	Enhanced by	1.000E+00		
O2	Enhanced by	8.200E-01		
NH3	Enhanced by	5.000E+00		
H2	Enhanced by	2.500E+00		
CO	Enhanced by	1.900E+00		
CO2	Enhanced by	3.800E+00		
18. H2O2+O=OH+HO2		9.640E+06	2.00	3970.0
19. H2O2+H=HO2+H2		4.820E+13	0.00	7948.0
20. H2O2+H=OH+H2O		2.410E+13	0.00	3975.0
21. H2O2+OH=H2O+HO2		1.000E+12	0.00	0.0
Declared duplicate reaction...				
22. H2O2+OH=H2O+HO2		5.800E+14	0.00	9557.0
Declared duplicate reaction...				
23. CH2O+O2=HCO+HO2		6.020E+13	0.00	40658.0
24. CH2O+O=HCO+OH		1.810E+13	0.00	3078.0
25. CH2O+H=HCO+H2		1.260E+08	1.62	2163.0
26. CH2O+OH=HCO+H2O		3.430E+09	1.18	-447.0
27. CH2O+HO2=HCO+H2O2		1.990E+12	0.00	11660.0
28. HCO+M=H+CO+M		1.850E+17	-1.00	17000.0
H2	Enhanced by	1.890E+00		
H2O	Enhanced by	1.200E+01		
CO	Enhanced by	1.900E+00		
CO2	Enhanced by	3.800E+00		
N2O	Enhanced by	5.000E+00		
29. HCO+O2=CO+HO2		7.580E+12	0.00	406.0
30. HCO+O=CO+OH		3.000E+13	0.00	0.0
31. HCO+O=CO2+H		3.000E+13	0.00	0.0
32. HCO+H=CO+H2		7.230E+13	0.00	0.0
33. HCO+OH=CO+H2O		3.000E+13	0.00	0.0
34. HCO+HO2=CO2+OH+H		3.000E+13	0.00	0.0
35. HCO+HCO=CH2O+CO		3.000E+13	0.00	0.0
36. HCO+HCO=H2+CO+CO		5.200E+12	0.00	0.0
37. CO+O(+M)=CO2(+M)		1.800E+10	0.00	2380.0
Low pressure limit:	0.13500E+25	-0.27880E+01	0.41910E+04	
TROE centering:	0.10000E+01	0.10000E-89	0.10000E+91	
N2	Enhanced by	1.330E+00		
H2	Enhanced by	2.500E+00		
H2O	Enhanced by	1.200E+01		
CO	Enhanced by	1.900E+00		
CO2	Enhanced by	3.800E+00		
N2O	Enhanced by	5.000E+00		
38. CO+O2=CO2+O		2.530E+12	0.00	47700.0
39. CO+OH=CO2+H		1.500E+07	1.30	-765.0
40. CO+HO2=CO2+OH		5.800E+13	0.00	22930.0
41. N+H2=NH+H		2.330E+14	0.00	30830.0
42. O+NO=N+O2		3.800E+09	1.00	41375.0
43. NO+H=N+OH		1.700E+14	0.00	48800.0
44. N+HO2=NH+O2		6.000E+12	0.00	0.0
45. N+HO2=NO+OH		1.000E+13	0.00	2000.0
46. N+NO=N2+O		3.270E+12	0.30	0.0
47. NO2+N=N2O+O		3.490E+12	0.00	-437.0
48. N+NO2=N2+O2		1.000E+12	0.00	0.0

49.	N+HNO=NH+NO		1.000E+13	0.00	2000.0	
50.	N+HNO=N2O+H		5.000E+10	0.50	3000.0	
51.	NO+M=N+O+M		9.640E+14	0.00	148400.0	
	N2	Enhanced by	1.500E+00			
	H2	Enhanced by	2.200E+00			
	H2O	Enhanced by	6.700E+00			
	N2O	Enhanced by	2.200E+00			
	CO2	Enhanced by	2.500E+00			
	NH3	Enhanced by	5.000E+00			
52.	NO+O(+M)=NO2(+M)		1.300E+15	-0.75	0.0	
	Low pressure limit:	0.47200E+25	-0.28700E+01	0.15510E+04		
	TROE centering:	0.95700E+00	0.10000E-89	0.83320E+04		
	N2O	Enhanced by	1.500E+00			
	H2O	Enhanced by	4.400E+00			
	N2	Enhanced by	1.000E+00			
	CO2	Enhanced by	2.300E+00			
	NH3	Enhanced by	5.000E+00			
53.	H+NO(+M)=HNO(+M)		1.520E+15	-0.41	0.0	
	Low pressure limit:	0.40000E+21	-0.17500E+01	0.00000E+00		
	N2O	Enhanced by	5.000E+00			
	H2O	Enhanced by	5.000E+00			
	N2	Enhanced by	1.000E+00			
	CO2	Enhanced by	1.300E+00			
	NH3	Enhanced by	5.000E+00			
54.	NO+OH(+M)=HONO(+M)		1.990E+12	-0.05	-721.0	
	Low pressure limit:	0.50800E+24	-0.25100E+01	-0.67560E+02		
	TROE centering:	0.62000E+00	0.10000E-89	0.10000E+91		
	N2O	Enhanced by	5.000E+00			
	H2O	Enhanced by	5.000E+00			
	N2	Enhanced by	1.000E+00			
	CO2	Enhanced by	1.300E+00			
	NH3	Enhanced by	5.000E+00			
55.	HO2+NO=OH+NO2	[3 atm]	2.350E+14	-0.67	46.0	
*	55.	HO2+NO=OH+NO2	[10 atm]	2.350E+14	-0.67	46.0
*	55.	HO2+NO=OH+NO2	[30 atm]	4.580E+14	-0.75	296.0
*	55.	HO2+NO=OH+NO2	[100 atm]	1.280E+15	-0.87	708.0
*	55.	HO2+NO=OH+NO2	[300 atm]	4.860E+15	-1.03	1349.0
*	55.	HO2+NO=OH+NO2	[1000 atm]	1.120E+16	-1.11	2148.0
56.	HO2+NO+M=HOONO+M	[3 atm]	8.010E+22	-3.08	369.0	
*	56.	HO2+NO+M=HOONO+M	[10 atm]	8.010E+22	-3.08	369.0
*	56.	HO2+NO=HOONO	[30 atm]	5.590E+22	-4.15	621.0
*	56.	HO2+NO=HOONO	[100 atm]	4.830E+23	-4.27	1029.0
*	56.	HO2+NO=HOONO	[300 atm]	4.420E+24	-4.39	1643.0
*	56.	HO2+NO=HOONO	[1000 atm]	1.910E+25	-4.41	2348.0
57.	HOONO+M=OH+NO2+M	[3 atm]	4.720E+30	-4.63	22453.0	
*	57.	HOONO+M=OH+NO2+M	[10 atm]	4.720E+30	-4.63	22453.0
*	57.	HOONO=OH+NO2	[30 atm]	5.190E+31	-6.01	24562.0
*	57.	HOONO=OH+NO2	[100 atm]	5.750E+31	-5.86	25109.0
*	57.	HOONO=OH+NO2	[300 atm]	1.210E+31	-5.51	25351.0
*	57.	HOONO=OH+NO2	[1000 atm]	3.360E+29	-4.91	25278.0
58.	NO+HCO=HNO+CO		7.230E+12	0.00	0.0	
59.	H2+NO2=HONO+H		1.300E+04	2.76	29770.0	
60.	HONO+H=HNO+OH		5.630E+10	0.86	4969.0	
61.	HONO+H=H2O+NO		8.130E+06	1.89	3847.0	
62.	NO2+O=O2+NO		3.910E+12	0.00	-238.0	
63.	NO2+O(+M)=NO3(+M)		1.330E+13	0.00	0.0	
	Low pressure limit:	0.14900E+29	-0.40800E+01	0.24670E+04		
	TROE centering:	0.82600E+00	0.10000E-89	0.31910E+04		
	N2O	Enhanced by	5.000E+00			
	H2O	Enhanced by	9.000E+00			
	CO2	Enhanced by	3.200E+00			
	O2	Enhanced by	8.200E-01			
64.	NO2+H=NO+OH		1.320E+14	0.00	361.6	
65.	NO2+OH(+M)=HNO3(+M)		2.410E+13	0.00	0.0	
	Low pressure limit:	0.64200E+33	-0.54900E+01	0.23500E+04		
	TROE centering:	0.83700E+00	0.10000E-89	0.16570E+04		
	N2O	Enhanced by	5.000E+00			
	H2O	Enhanced by	9.000E+00			
	CO2	Enhanced by	3.200E+00			
	O2	Enhanced by	8.200E-01			
66.	NO2+CH2O=HONO+HCO		8.020E+02	2.77	13730.0	

67.	NO2+HCO=CO+HONO		1.240E+23	-3.29	2354.0
68.	NO2+HCO=H+CO2+NO		8.390E+15	-0.75	1927.0
69.	NO2+CO=CO2+NO		9.030E+13	0.00	33780.0
70.	NO2+NO2=NO3+NO		9.640E+09	0.73	20920.0
71.	NO2+NO2=NO+NO+O2		4.510E+12	0.00	27600.0
72.	NH+M=N+H+M		5.100E+14	0.00	79720.0
	N2O	Enhanced by	5.000E+00		
	H2O	Enhanced by	9.000E+00		
	O2	Enhanced by	8.200E-01		
	NH3	Enhanced by	5.000E+00		
73.	NH+O2=HNO+O		4.610E+05	2.00	6500.0
74.	NH+O2=NO+OH		1.280E+06	1.50	100.0
75.	NH+O2=H+NO2		2.300E+10	0.00	2484.0
76.	NH+O=NO+H		5.500E+13	0.00	0.0
77.	NH+O=N+OH		3.720E+13	0.00	0.0
78.	NH+OH=N+H2O		1.200E+06	2.00	-487.0
79.	NH+OH=HNO+H		2.000E+13	0.00	0.0
80.	NH2+O=HNO+H		4.600E+13	0.00	0.0
81.	NH2+O=NH+OH		7.000E+12	0.00	0.0
	Declared duplicate reaction...				
82.	NH2+O=NH+OH		3.330E+08	1.50	5077.0
	Declared duplicate reaction...				
83.	NH+N=N2+H		3.000E+13	0.00	0.0
84.	NH+NO2=N2O+OH		4.000E+12	0.00	0.0
85.	NH+NO2=NO+HNO		5.700E+12	0.00	0.0
86.	NH+NH=N2+H+H		5.100E+13	0.00	0.0
87.	NH2+O2=NH2O+O		2.500E+11	0.48	29586.0
88.	NH2+O2=HNO+OH		6.200E+07	1.23	35100.0
89.	NH2+H=NH+H2		4.000E+13	0.00	3650.0
90.	NH2+N=N2+2H		7.200E+13	0.00	0.0
91.	NH2+NO=HNO+NH		1.000E+13	0.00	40000.0
92.	NO2+NH2=N2O+H2O		1.540E+16	-1.44	268.0
93.	NO2+NH2=NH2O+NO		6.560E+16	-1.44	268.0
94.	NH3 (+M)=NH2+H (+M)		5.500E+15	0.00	107792.0
	Low pressure limit: 0.22000E+17 0.00000E+00 0.93470E+05				
	N2O	Enhanced by	5.000E+00		
	H2O	Enhanced by	9.000E+00		
	CO2	Enhanced by	3.200E+00		
	O2	Enhanced by	8.200E-01		
95.	NH3+O=NH2+OH		9.400E+06	1.94	6460.0
96.	NH3+H=NH2+H2		6.400E+05	2.39	10170.0
97.	NH3+OH=NH2+H2O		2.040E+06	2.04	566.0
98.	NH2+H2O2=NH3+HO2		9.200E+05	1.94	4000.0
99.	NH2+HO2=NH2O+OH		2.500E+13	0.00	0.0
100.	NH2+HO2=NH3+O2		9.200E+05	1.94	-1152.0
101.	NNH (+M)=N2+H (+M)		4.100E+09	1.13	5186.0
	Low pressure limit: 0.10000E+14 0.50000E+00 0.30600E+04				
	N2O	Enhanced by	5.000E+00		
	H2O	Enhanced by	9.000E+00		
	O2	Enhanced by	8.200E-01		
	CO2	Enhanced by	3.200E+00		
	NH3	Enhanced by	5.000E+00		
	Declared duplicate reaction...				
102.	NNH=N2+H		3.000E+08	0.00	0.0
	Declared duplicate reaction...				
103.	NNH+H=N2+H2		2.400E+08	1.50	-894.0
104.	NNH+OH=N2+H2O		2.400E+22	-2.88	2454.0
	Declared duplicate reaction...				
105.	NNH+OH=N2+H2O		1.200E+06	2.00	-1192.0
	Declared duplicate reaction...				
106.	NNH+NO=HNO+N2		1.200E+06	2.00	-1192.0
107.	NNH+NH=N2+NH2		5.000E+13	0.00	0.0
108.	NNH+NH2=N2+NH3		9.200E+05	1.94	-1152.0
109.	HNO+O2=NO+HO2		2.000E+13	0.00	15896.0
110.	HNO+O=OH+NO		3.610E+13	0.00	0.0
111.	H+HNO=H2+NO		4.460E+11	0.72	655.0
112.	HNO+OH=NO+H2O		1.295E+07	1.88	-958.0
113.	HNO+HCO=CH2O+NO		6.020E+11	0.00	1987.0
114.	HNO+NO=N2O+OH		1.700E+13	0.00	29590.0
115.	HNO+NO2=HONO+NO		4.420E+04	2.64	4042.0
116.	HNO+NH2=NH3+NO		9.200E+05	1.94	-1152.0

117.	HNO+HNO=N2O+H2O		3.630E-03	3.98	1190.0
118.	HONO+O=OH+NO2		1.700E+08	1.50	3030.0
119.	HONO+OH=H2O+NO2		1.200E+06	2.00	-596.0
120.	HONO+HNO=H2O+2NO		3.100E+10	0.00	21400.0
121.	NH3+HONO=NH2NO+H2O		1.000E-03	4.25	29600.0
122.	HCN(+M)=H+CN(+M)		8.300E+17	-0.93	123800.0
	Low pressure limit:	0.35700E+27	-0.26000E+01	0.12490E+06	
	TROE centering:	0.95700E+00	0.10000E-89	0.83320E+04	
	N2O	Enhanced by	5.000E+00		
	H2O	Enhanced by	9.000E+00		
	CO2	Enhanced by	3.200E+00		
	O2	Enhanced by	8.200E-01		
123.	HCN+O=CN+OH		2.700E+09	1.58	26600.0
124.	HCN+O=NH+CO		3.450E+03	2.64	4980.0
125.	HCN+O=NCO+H		1.380E+04	2.64	4980.0
126.	HCN+OH=H2O+CN		3.900E+06	1.83	10290.0
127.	HCN+OH=H+HNCO		1.980E-03	4.00	1000.0
128.	HCN+OH=NH2+CO		7.830E-04	4.00	4000.0
129.	HCN+M=HNC+M		1.560E+26	-3.23	49576.0
	AR	Enhanced by	7.000E-01		
	H2O	Enhanced by	7.000E+00		
	CO2	Enhanced by	2.000E+00		
	N2O	Enhanced by	5.000E+00		
	O2	Enhanced by	8.200E-01		
130.	HNC+O=NH+CO		5.440E+12	0.00	0.0
131.	HNC+O=H+NCO		1.600E+01	3.08	-224.0
132.	HNC+OH=HNCO+H		2.800E+13	0.00	3700.0
133.	HNC+OH=CN+H2O		1.500E+12	0.00	7680.0
134.	HNC+NO2=HNCO+NO		1.000E+12	0.00	32000.0
135.	HNC+CN=C2N2+H		1.000E+13	0.00	0.0
136.	N2O(+M)=N2+O(+M)		1.260E+12	0.00	62620.0
	Low pressure limit:	0.59700E+15	0.00000E+00	0.56640E+05	
	N2O	Enhanced by	5.000E+00		
	H2O	Enhanced by	9.000E+00		
	N2	Enhanced by	1.000E+00		
	CO2	Enhanced by	3.200E+00		
	O2	Enhanced by	8.200E-01		
	AR	Enhanced by	6.700E-01		
137.	N2O+O=N2+O2		3.692E+12	0.00	15940.0
138.	N2O+O=NO+NO		9.155E+13	0.00	27680.0
139.	N2O+OH=N2+HO2		1.290E-02	4.72	36561.0
140.	N2O+NO=N2+NO2		4.290E+13	0.00	47130.0
141.	NO+NO+NO=N2O+NO2		1.070E+10	0.00	26800.0
142.	CN+H2=H+HCN		5.500E+02	3.18	-223.0
143.	CN+O2=NCO+O		7.500E+12	0.00	-389.0
144.	CN+O=CO+N		1.800E+13	0.00	0.0
145.	CN+OH=NCO+H		4.220E+13	0.00	0.0
146.	CN+CH2O=HCN+HCO		4.220E+13	0.00	0.0
147.	CN+HCO=HCN+CO		6.020E+13	0.00	0.0
148.	CN+CO2=CO+NCO		3.670E+06	2.16	26900.0
149.	CN+NO=NCO+N		5.500E+12	0.00	30620.0
150.	CN+NO=N2+CO		3.900E+11	0.00	27820.0
151.	CN+NO=NCN+O		1.800E+13	0.00	38190.0
152.	CN+NO2=NCO+NO		1.590E+13	0.00	-1133.0
153.	CN+HNO=HCN+NO		1.810E+13	0.00	0.0
154.	CN+HONO=HCN+NO2		1.200E+13	0.00	0.0
155.	CN+HCN=H+C2N2		1.210E+07	1.71	1530.0
156.	CN+N2O=NCN+NO		2.400E+13	0.00	13330.0
157.	CN+NH3=HCN+NH2		9.200E+12	0.00	-358.0
158.	CN+CN(+M)=C2N2(+M)		5.660E+12	0.00	0.0
	Low pressure limit:	0.34200E+26	-0.26100E+01	0.00000E+00	
	TROE centering:	0.50000E+00	0.10000E-89	0.10000E+91	
	N2O	Enhanced by	5.000E+00		
	H2O	Enhanced by	9.000E+00		
	CO2	Enhanced by	3.200E+00		
	O2	Enhanced by	8.200E-01		
159.	C2N2+O=NCO+CN		4.570E+12	0.00	8880.0
160.	NCN+O2=NO+NCO		1.000E+14	0.00	0.0
161.	NCN+H=HCN+N		1.000E+14	0.00	0.0
162.	NCN+H=CN+NH		5.000E+14	0.00	30000.0
163.	NCO+M=N+CO+M		1.140E+23	-1.95	59930.0



N2O	Enhanced by	5.000E+00		
H2O	Enhanced by	5.000E+00		
N2	Enhanced by	1.000E+00		
CO2	Enhanced by	1.500E+00		
164. NCO+H2=HNCO+H		7.600E+02	3.00	4000.0
165. NCO+O2=NO+CO2		2.000E+12	0.00	20000.0
166. NCO+O=CO+NO		2.000E+13	0.00	0.0
167. NCO+H=NH+CO		5.360E+13	0.00	0.0
168. NCO+OH=NO+CO+H		2.000E+13	0.00	7500.0
169. NCO+OH=NO+HCO		5.000E+12	0.00	15000.0
170. NCO+CH2O=HNCO+HCO		6.020E+12	0.00	0.0
171. NCO+HCO=HNCO+CO		3.610E+13	0.00	0.0
172. NCO+N=N2+CO		2.000E+13	0.00	0.0
173. NCO+NO=N2O+CO		3.980E+19	-2.19	1743.0
174. NCO+NO=CO2+N2		1.460E+21	-2.74	1824.0
175. NCO+NO2=CO2+N2O		1.950E+13	-0.26	-620.0
176. NCO+NO2=CO+NO+NO		1.770E+12	-0.26	-620.0
177. NCO+HNO=HNCO+NO		1.810E+13	0.00	0.0
178. NCO+HONO=HNCO+NO2		3.610E+12	0.00	0.0
179. NCO+N2O=N2+NO+CO		9.030E+13	0.00	27820.0
180. NCO+CN=NCN+CO		1.810E+13	0.00	0.0
181. NCO+NCO=N2+2CO		1.000E+13	0.00	0.0
182. CNO+O=CO+NO		1.000E+13	0.00	0.0
183. CNO+NO2=CO+2NO		1.000E+13	0.00	0.0
184. CNO+N2O=N2+CO+NO		1.000E+12	0.00	15000.0
185. HNCO(+M)=NH+CO(+M)		6.000E+13	0.00	99800.0
Low pressure limit:	0.21700E+29	-0.31000E+01	0.10190E+06	
TROE centering:	0.93800E+00	0.10000E-89	0.33040E+04	
N2O	Enhanced by	5.000E+00		
H2O	Enhanced by	9.000E+00		
CO2	Enhanced by	3.200E+00		
O2	Enhanced by	8.200E-01		
186. HNCO+O2=HNO+CO2		1.000E+12	0.00	35000.0
187. HNCO+O=CO2+NH		9.640E+07	1.41	8524.0
188. HNCO+O=OH+NCO		2.200E+06	2.11	11430.0
189. HNCO+O=HNO+CO		1.580E+08	1.57	44300.0
190. HNCO+H=NH2+CO		2.200E+07	1.70	3800.0
191. HNCO+OH=H2O+NCO		4.790E+05	2.00	2560.0
192. HNCO+OH=NH2+CO2		1.600E+05	2.00	2560.0
193. HNCO+HO2=NCO+H2O2		3.000E+11	0.00	23700.0
194. HNCO+NH=NH2+NCO		2.000E+13	0.00	19300.0
195. HOCN+NH2=NCO+NH3		9.200E+05	1.94	3646.0
196. NCO+NH3=HNCO+NH2		2.770E+04	2.48	981.0
197. HNCO+CN=HCN+NCO		1.510E+13	0.00	0.0
198. HCNO+H=HNCO+H		2.100E+15	-0.69	2851.0
199. HCNO+H=HCN+OH		2.700E+11	0.18	2116.0
200. HCNO+H=NH2+CO		1.700E+14	-0.75	2891.0
201. HCNO+H=HOCN+H		1.400E+11	-0.19	2484.0
202. HCNO+O=HCO+NO		1.000E+12	0.00	9000.0
203. HCNO+OH=HCO+HNO		1.000E+13	0.00	5000.0
204. HCNO+OH=CNO+H2O		1.000E+12	0.00	2000.0
205. HCNO+CN=HCN+CNO		1.000E+12	0.00	2000.0
206. HOCN+O=NCO+OH		1.500E+04	2.64	4000.0
207. OH+HCN=HOCN+H		1.100E+06	2.03	13373.0
208. HOCN+H=HNCO+H		3.100E+08	0.84	1917.0
209. HOCN+H=NH2+CO		1.200E+08	0.61	2076.0
210. HOCN+H=H2+NCO		2.400E+08	1.50	6617.0
211. HOCN+OH=NCO+H2O		6.400E+05	2.00	2560.0
212. H2CN+M=HCN+H+M		5.300E+16	0.00	29000.0
N2O	Enhanced by	5.000E+00		
H2O	Enhanced by	9.000E+00		
CO2	Enhanced by	3.200E+00		
O2	Enhanced by	8.200E-01		
213. H2CN+CH2O=H2CNH+HCO		1.000E+11	0.00	14000.0
214. H2CN+NO=HCN+HNO		1.000E+11	0.00	3000.0
215. H2CN+NO2=HCN+HONO		1.000E+11	0.00	1000.0
216. H2CN+NO2=H2CNO+NO		1.000E+11	0.00	3000.0
217. H2CN+HNO=H2CNH+NO		1.000E+11	0.00	4000.0
218. H2CN+HONO=H2CNH+NO2		1.000E+11	0.00	12000.0
219. H2CN+N2O=H2CNO+N2		1.000E+11	0.00	3000.0
220. H2CN+N=HCN+NH		7.200E+13	0.00	400.0

221.	H2CN+H=HCN+H2	4.000E+13	0.00	0.0
222.	H2CN+OH=HCN+H2O	2.000E+13	0.00	0.0
223.	H2CNH+OH=H2CN+H2O	1.000E+13	0.00	0.0
224.	H2CNH+CN=H2CN+HCN	1.000E+13	0.00	0.0
225.	H2CNO+M=HCNO+H	1.000E+16	0.00	50000.0
226.	H2CNO+OH=HCNO+H2O	1.000E+13	0.00	0.0
227.	H2CNO+NO=HCNO+HNO	1.000E+12	0.00	25000.0
228.	H2CNO+NO2=HCNO+HONO	1.000E+12	0.00	2000.0
229.	H2CNO+NO2=CH2O+NO+NO	1.000E+12	0.00	0.0
230.	H2CNO+HNO=H2CN+HONO	1.000E+12	0.00	2000.0
231.	H2CNNO(+M)=H2CN+NO(+M)	1.000E+16	0.00	20000.0
	Low pressure limit: 0.76900E+17 0.00000E+00 0.15000E+05			
232.	H2CNNO2(+M)=H2CN+NO2(+M)	1.000E+16	0.00	31000.0
	Low pressure limit: 0.76900E+17 0.00000E+00 0.26000E+05			
233.	H2CNNO2+H2O=CH2O+N2O+H2O	1.000E+11	0.00	2000.0
234.	H2CNNO2+NO2=CH2O+N2O+NO2	1.000E+11	0.00	2000.0
235.	H2CNNO2+N2O=CH2O+N2O+N2O	1.000E+11	0.00	2000.0
236.	H2CNNO2+H=H2CN+HONO	1.000E+12	0.00	5000.0
237.	H2CNNO2+OH=HCN+NO2+H2O	1.000E+13	0.00	3000.0
238.	H2CNNO2+OH=CH2O+N2O+OH	1.000E+13	0.00	0.0
239.	RDX(+M)=RDXR+NO2(+M)	2.000E+16	0.00	45000.0
	Low pressure limit: 0.15700E+18 0.00000E+00 0.28000E+05			
240.	RDX+H=RDXR+HONO	1.000E+13	0.00	5000.0
241.	RDX+OH=>2H2CNNO2+H2COHNO2	1.000E+13	0.00	5000.0
242.	H2COHNO2=>HCN+NO2+H2O	1.000E+16	0.00	0.0
243.	RDXR(+M)=>RDXRO(+M)	1.000E+16	0.00	23000.0
	Low pressure limit: 0.76900E+17 0.00000E+00 0.18000E+05			
244.	RDXRO(+M)=>2H2CNNO2+H2CN(+M)	1.000E+16	0.00	23000.0
	Low pressure limit: 0.76900E+17 0.00000E+00 0.18000E+05			
245.	HONO+NH2=NO2+NH3	1.000E+10	1.00	0.0
246.	NO2+NO3=NO+NO2+O2	2.710E+10	0.00	2500.0
247.	H2NN+O2=NH2+NO2	1.500E+12	0.00	5961.0
248.	H2NN+H=NNH+H2	4.800E+08	1.50	-894.0
249.	H2NN+H=N2H2+H	1.830E+10	0.97	4471.0
250.	H2NN+O=NNH+OH	3.300E+08	1.50	-894.0
251.	H2NN+O=NH2+NO	3.180E+09	1.03	2695.0
252.	H2NN+OH=NNH+H2O	2.400E+06	2.00	-1192.0
253.	H2NN+OH=NH2NO+H	2.000E+12	0.00	0.0
254.	H2NN+HO2=NH2NO+OH	6.560E+05	1.94	7053.0
255.	H2NN+HO2=NNH+H2O2	2.900E+04	2.69	-1600.0
256.	H2NN+NH2=HNNNH2+H	7.880E+06	1.90	-1333.0
257.	H2NN+NH2=NNH+NH3	1.800E+06	1.94	-1152.0
258.	N2H3+H=N2H2+H2	2.400E+08	1.50	-10.0
259.	N2H3+O=NH2+HNO	3.000E+13	0.00	0.0
260.	N2H3+O=NH2NO+H	3.000E+13	0.00	0.0
261.	N2H3+O=N2H2+OH	1.700E+08	1.50	-646.0
262.	N2H3+OH=N2H2+H2O	1.200E+06	2.00	-1192.0
263.	N2H3+OH=H2NN+H2O	3.000E+13	0.00	0.0
264.	N2H3+NH2=N2H2+NH3	9.200E+05	1.94	-1152.0
265.	N2H3+NH2=H2NN+NH3	3.000E+13	0.00	0.0
266.	N2H3+HO2=H2NNHO+OH	3.000E+13	0.00	0.0
267.	N2H3+HO2=N2H2+H2O2	2.900E+04	2.69	-1600.0
268.	N2H3+HO2=N2H4+O2	9.200E+05	1.94	2126.0
269.	N2H3+N2H3=2NH3+N2	3.000E+12	0.00	0.0
270.	N2H3+N2H3=N2H4+N2H2	1.200E+13	0.00	0.0
271.	N2H4+H=N2H3+H2	4.900E+12	0.00	2130.0
272.	N2H4+O=N2H3+OH	6.700E+08	1.50	2851.0
273.	N2H4+OH=N2H3+H2O	4.800E+06	2.00	-646.0
274.	N2H4+NH2=N2H3+NH3	1.800E+06	1.71	-1380.0
275.	N2H2+H=NNH+H2	8.490E+04	2.63	-230.0
276.	N2H2+O=NNH+OH	3.300E+08	1.50	497.0
277.	N2H2+OH=NNH+H2O	5.930E+01	3.40	-1360.0
278.	N2H2+NH2=NH3+NNH	8.790E-02	4.05	-1610.0
279.	N2H2+NH=NNH+NH2	2.400E+06	2.00	-1192.0
280.	N2H2+NO=N2O+NH2	4.000E+12	0.00	11922.0
281.	NH2NO+H=HNNO+H2	4.800E+08	1.50	7412.0
282.	NH2NO+O=HNNO+OH	3.300E+08	1.50	4699.0
283.	NH2NO+OH=HNNO+H2O	2.400E+06	2.00	-70.0
284.	NH2NO+CH3=HNNO+CH4	1.600E+06	1.87	7183.0
285.	NH2NO+NH2=HNNO+NH3	1.800E+06	1.94	4540.0
286.	NH2NO+HO2=HNNO+H2O2	2.900E+04	2.69	12627.0

287.	NH2O+M=HNO+H+M		2.790E+24	-2.83	64915.0
	N2O	Enhanced by	5.000E+00		
	H2O	Enhanced by	7.000E+00		
	N2	Enhanced by	1.000E+00		
	O2	Enhanced by	8.200E-01		
	HNO3	Enhanced by	5.000E+00		
	NH3	Enhanced by	5.000E+00		
	NO3	Enhanced by	5.000E+00		
288.	NH2O+M=HNOH+M		1.070E+29	-3.99	43982.0
	N2O	Enhanced by	5.000E+00		
	H2O	Enhanced by	7.000E+00		
	N2	Enhanced by	1.000E+00		
	O2	Enhanced by	8.200E-01		
	HNO3	Enhanced by	5.000E+00		
	NH3	Enhanced by	5.000E+00		
	NO3	Enhanced by	5.000E+00		
289.	NH2O+H=NH2+OH		4.000E+13	0.00	0.0
290.	NH2O+H=HNO+H2		4.800E+08	1.50	1560.0
291.	NH2O+O=HNO+OH		3.300E+08	1.50	487.0
292.	NH2O+OH=HNO+H2O		2.400E+06	2.00	-1192.0
293.	NH2O+NH2=HNO+NH3		1.800E+06	1.94	-1152.0
294.	NH2O+HO2=HNO+H2O2		2.900E+04	2.69	-1600.0
295.	NH2O+HO2=NH2OH+O2		2.900E+04	2.69	-1600.0
296.	HNOH+M=H+HNO+M		1.970E+24	-2.84	58934.0
	N2O	Enhanced by	5.000E+00		
	H2O	Enhanced by	7.000E+00		
	N2	Enhanced by	1.000E+00		
	O2	Enhanced by	8.200E-01		
	HNO3	Enhanced by	5.000E+00		
	NH3	Enhanced by	5.000E+00		
	NO3	Enhanced by	5.000E+00		
297.	HNOH+H=NH2+OH		4.000E+13	0.00	0.0
298.	HNOH+H=HNO+H2		4.800E+08	1.50	378.0
299.	HNOH+O=HNO+OH		7.000E+13	0.00	0.0
	Declared duplicate reaction...				
300.	HNOH+O=HNO+OH		3.300E+08	1.50	-358.0
	Declared duplicate reaction...				
301.	HNOH+OH=HNO+H2O		2.400E+06	2.00	-1192.0
302.	HNOH+NH2=HNO+NH3		1.800E+06	1.94	-1152.0
303.	HNOH+NH2=N2H3+OH		6.720E+06	1.82	715.0
304.	HNOH+NH2=H2NN+H2O		4.570E+19	-1.94	1927.0
305.	HNOH+HO2=HONHO+OH		4.000E+13	0.00	0.0
306.	HNOH+HO2=HNO+H2O2		2.900E+04	2.69	-1600.0
307.	HNOH+HO2=NH2OH+O2		2.900E+04	2.69	-1600.0
308.	HNOO+M=OH+NO+M		1.520E+36	-6.18	31131.0
	N2O	Enhanced by	5.000E+00		
	H2O	Enhanced by	7.000E+00		
	N2	Enhanced by	1.000E+00		
	O2	Enhanced by	8.200E-01		
	HNO3	Enhanced by	5.000E+00		
	NH3	Enhanced by	5.000E+00		
	NO3	Enhanced by	5.000E+00		
309.	HNO2+H=H2+NO2		2.400E+08	1.50	4163.0
310.	HNO2+O=OH+NO2		1.700E+08	1.50	2365.0
311.	HNO2+OH=H2O+NO2		1.200E+06	2.00	-795.0
312.	HNO2+NH2=NO2+NH3		9.200E+05	1.94	874.0
313.	HON+M=NO+H+M		5.090E+19	-1.73	16045.0
	N2O	Enhanced by	5.000E+00		
	H2O	Enhanced by	7.000E+00		
	N2	Enhanced by	1.000E+00		
	O2	Enhanced by	8.200E-01		
	HNO3	Enhanced by	5.000E+00		
	NH3	Enhanced by	5.000E+00		
	NO3	Enhanced by	5.000E+00		
314.	HON+H=HNO+H		2.000E+13	0.00	0.0
315.	HON+H=OH+NH		2.000E+13	0.00	0.0
316.	HON+O=OH+NO		7.000E+13	0.00	0.0
317.	HON+OH=HONO+H		4.000E+13	0.00	0.0
318.	HON+O2=HONO+O		1.000E+12	0.00	4968.0
319.	NH2OH+H=HNOH+H2		4.800E+08	1.50	6249.0
320.	NH2OH+H=NH2O+H2		2.400E+08	1.50	5067.0

321.	NH2OH+O=HNOH+OH	3.300E+08	1.50	3865.0
322.	NH2OH+O=NH2O+OH	1.700E+08	1.50	3010.0
323.	NH2OH+OH=HNOH+H2O	2.400E+06	2.00	-328.0
324.	NH2OH+OH=NH2O+H2O	1.200E+06	2.00	-596.0
325.	NH2OH+NH2=HNOH+NH3	1.800E+06	1.94	3229.0
326.	NH2OH+NH2=NH2O+NH3	9.200E+05	1.94	1888.0
327.	NH2OH+HO2=HNOH+H2O2	2.900E+04	2.69	9557.0
328.	NH2OH+HO2=NH2O+H2O2	1.400E+04	2.69	6418.0
329.	H2NNHO+H=HNNHO+H2	4.800E+08	1.50	-894.0
330.	H2NNHO+O=HNNHO+OH	3.300E+08	1.50	-894.0
331.	H2NNHO+OH=HNNHO+H2O	2.400E+06	2.00	-1192.0
332.	H2NNHO+CH3=HNNHO+CH4	1.600E+06	1.87	378.0
333.	H2NNHO+NH2=HNNHO+NH3	1.800E+06	1.94	-1152.0
334.	H2NNHO+HO2=HNNHO+H2O2	2.900E+04	2.69	-1600.0
335.	HNCO+NO2=HNNO+CO2	2.500E+12	0.00	26000.0
336.	HNO+NO+NO=HNNO+NO2	1.700E+11	0.00	2100.0
337.	HNNO+NO=NNH+NO2	3.200E+12	0.00	270.0
338.	HNNO+NO=N2+HONO	2.600E+11	0.00	810.0
339.	HNNO+OH=H2O+N2O	2.000E+13	0.00	0.0
340.	HNNO+H=H2+N2O	2.000E+13	0.00	0.0
341.	HNNO+O=N2O+OH	2.000E+13	0.00	0.0
342.	HNNO+HO2=H2O2+N2O	1.500E+12	0.00	2000.0
343.	HNNO+NH2=NH3+N2O	1.000E+12	0.00	0.0
344.	HNNO+NO2=HONO+N2O	1.000E+12	0.00	0.0
345.	H+N2O=N2+OH	1.500E+11	1.00	18400.0
Declared duplicate reaction...				
346.	H+N2O=N2+OH [3 atm]	1.270E+16	-0.86	14609.0
*346.	H+N2O=N2+OH [10 atm]	2.880E+16	-0.96	14960.0
*346.	H+N2O=N2+OH [30 atm]	8.220E+16	-1.08	15520.0
*346.	H+N2O=N2+OH [100 atm]	1.150E+17	-1.10	16203.0
*346.	H+N2O=N2+OH [300 atm]	1.810E+16	-0.85	16564.0
*346.	H+N2O=N2+OH [1000 atm]	1.110E+14	-0.21	16440.0
Declared duplicate reaction...				
347.	H+N2O=HNNO [3 atm]	5.510E+28	-5.32	12100.0
*347.	H+N2O=HNNO [10 atm]	2.510E+29	-5.35	12707.0
*347.	H+N2O=HNNO [30 atm]	1.720E+29	-5.15	13089.0
*347.	H+N2O=HNNO [100 atm]	9.180E+27	-4.63	13108.0
*347.	H+N2O=HNNO [300 atm]	9.160E+25	-3.93	12759.0
*347.	H+N2O=HNNO [1000 atm]	1.640E+23	-3.02	12083.0
348.	H+N2O=O+NNH [3 atm]	5.970E+19	-1.43	47174.0
*348.	H+N2O=O+NNH [10 atm]	5.970E+19	-1.43	47174.0
*348.	H+N2O=O+NNH [30 atm]	5.970E+19	-1.43	47174.0
*348.	H+N2O=O+NNH [100 atm]	5.970E+19	-1.43	47174.0
*348.	H+N2O=O+NNH [300 atm]	5.970E+19	-1.43	47174.0
*348.	H+N2O=O+NNH [1000 atm]	1.340E+20	-1.52	47540.0
349.	NH+NO=H+N2O [3 atm]	1.330E+19	-1.88	1526.0
*349.	NH+NO=H+N2O [10 atm]	1.330E+19	-1.88	1526.0
*349.	NH+NO=H+N2O [30 atm]	1.330E+19	-1.88	1526.0
*349.	NH+NO=H+N2O [100 atm]	2.610E+19	-1.96	1823.0
*349.	NH+NO=H+N2O [300 atm]	5.410E+19	-2.04	2209.0
*349.	NH+NO=H+N2O [1000 atm]	8.680E+19	-2.09	2804.0
350.	NH+NO=N2+OH [3 atm]	1.010E+18	-1.71	1409.0
*350.	NH+NO=N2+OH [10 atm]	1.010E+18	-1.71	1409.0
*350.	NH+NO=N2+OH [30 atm]	1.010E+18	-1.71	1409.0
*350.	NH+NO=N2+OH [100 atm]	2.000E+18	-1.79	1707.0
*350.	NH+NO=N2+OH [300 atm]	4.190E+18	-1.87	2095.0
*350.	NH+NO=N2+OH [1000 atm]	6.980E+18	-1.92	2696.0
351.	NH+NO=O+NNH [3 atm]	4.650E+11	0.54	11224.0
*351.	NH+NO=O+NNH [10 atm]	4.650E+11	0.54	11224.0
*351.	NH+NO=O+NNH [30 atm]	4.650E+11	0.54	11224.0
*351.	NH+NO=O+NNH [100 atm]	4.650E+11	0.54	11224.0
*351.	NH+NO=O+NNH [300 atm]	4.650E+11	0.54	11224.0
*351.	NH+NO=O+NNH [1000 atm]	1.080E+12	0.44	11626.0
352.	NH+NO+M=HNNO+M [3 atm]	4.430E+25	-3.52	2063.0
*352.	NH+NO+M=HNNO+M [10 atm]	4.430E+25	-3.52	2063.0
*352.	NH+NO+M=HNNO+M [30 atm]	4.430E+25	-3.52	2063.0
*352.	NH+NO=HNNO [100 atm]	1.040E+26	-4.60	2358.0
*352.	NH+NO=HNNO [300 atm]	6.280E+26	-4.68	2740.0
*352.	NH+NO=HNNO [1000 atm]	3.070E+27	-4.71	3318.0
353.	HNNO=N2+OH [3 atm]	3.640E+24	-4.48	31858.0
*353.	HNNO=N2+OH [10 atm]	2.540E+25	-4.57	32206.0

*353.	HNNO=N2+OH	[30 atm]	1.670E+26	-4.65	32734.0
*353.	HNNO=N2+OH	[100 atm]	3.890E+26	-4.59	33305.0
*353.	HNNO=N2+OH	[300 atm]	7.140E+25	-4.23	33489.0
*353.	HNNO=N2+OH	[1000 atm]	6.010E+23	-3.49	33169.0
354.	HNNO+M=O+NNH+M	[3 atm]	2.360E+25	-3.02	63996.0
*354.	HNNO+M=O+NNH+M	[10 atm]	2.360E+25	-3.02	63996.0
*354.	HNNO+M=O+NNH+M	[30 atm]	2.360E+25	-3.02	63996.0
*354.	HNNO+M=O+NNH+M	[100 atm]	2.360E+25	-3.02	63996.0
*354.	HNNO+M=O+NNH+M	[300 atm]	2.360E+25	-3.02	63996.0
*354.	HNNO=O+NNH	[1000 atm]	6.380E+26	-4.11	64361.0
355.	NH2+OH=NH2OH	[3 atm]	2.460E+40	-8.71	8331.0
*355.	NH2+OH=NH2OH	[10 atm]	1.560E+41	-8.77	9372.0
*355.	NH2+OH=NH2OH	[30 atm]	1.160E+41	-8.58	10056.0
*355.	NH2+OH=NH2OH	[100 atm]	1.560E+41	-8.77	9372.0
*355.	NH2+OH=NH2OH	[300 atm]	1.160E+41	-8.58	10056.0
*355.	NH2+OH=NH2OH	[1000 atm]	6.150E+39	-8.06	10276.0
356.	NH2+OH=NH+H2O		2.400E+06	2.00	50.0
357.	NH2+NH=NH3+N		9.200E+05	1.94	2444.0
358.	NH2+NH=N2H3	[3 atm]	5.280E+32	-6.94	4612.0
*358.	NH2+NH=N2H3	[10 atm]	2.140E+33	-6.96	4700.0
*358.	NH2+NH=N2H3	[30 atm]	1.070E+34	-7.02	4935.0
*358.	NH2+NH=N2H3	[100 atm]	1.400E+35	-7.18	5587.0
*358.	NH2+NH=N2H3	[300 atm]	3.300E+36	-7.41	6708.0
*358.	NH2+NH=N2H3	[1000 atm]	5.130E+37	-7.57	8162.0
359.	NH2+NH=N2H2+H	[3 atm]	1.450E+21	-2.51	1825.0
*359.	NH2+NH=N2H2+H	[10 atm]	1.770E+21	-2.53	1913.0
*359.	NH2+NH=N2H2+H	[30 atm]	2.960E+21	-2.59	2146.0
*359.	NH2+NH=N2H2+H	[100 atm]	1.200E+22	-2.75	2798.0
*359.	NH2+NH=N2H2+H	[300 atm]	1.060E+23	-3.00	3938.0
*359.	NH2+NH=N2H2+H	[1000 atm]	7.380E+23	-3.21	5482.0
360.	NH2+NH=H2+NNH	[3 atm]	1.080E+17	-1.13	1678.0
*360.	NH2+NH=H2+NNH	[10 atm]	1.320E+17	-1.15	1766.0
*360.	NH2+NH=H2+NNH	[30 atm]	2.220E+17	-1.21	1998.0
*360.	NH2+NH=H2+NNH	[100 atm]	8.960E+17	-1.38	2650.0
*360.	NH2+NH=H2+NNH	[300 atm]	8.010E+18	-1.63	3792.0
*360.	NH2+NH=H2+NNH	[1000 atm]	5.840E+19	-1.84	5344.0
361.	N2H3=N2H2+H	[3 atm]	5.250E+43	-9.40	57787.0
*361.	N2H3=N2H2+H	[10 atm]	8.840E+42	-9.03	58256.0
*361.	N2H3=N2H2+H	[30 atm]	3.650E+41	-8.50	58314.0
*361.	N2H3=N2H2+H	[100 atm]	1.170E+39	-7.66	57801.0
*361.	N2H3=N2H2+H	[300 atm]	7.820E+35	-6.66	56764.0
*361.	N2H3=N2H2+H	[1000 atm]	5.340E+31	-5.37	55140.0
362.	N2H3=H2+NNH	[3 atm]	9.010E+38	-7.95	58890.0
*362.	N2H3=H2+NNH	[10 atm]	4.880E+39	-7.98	60151.0
*362.	N2H3=H2+NNH	[30 atm]	1.400E+39	-7.67	60769.0
*362.	N2H3=H2+NNH	[100 atm]	1.180E+37	-6.92	60625.0
*362.	N2H3=H2+NNH	[300 atm]	1.060E+34	-5.93	59778.0
*362.	N2H3=H2+NNH	[1000 atm]	6.150E+29	-4.62	58221.0
363.	NH2+NO=NNH+OH	[3 atm]	2.290E+10	0.42	-815.0
*363.	NH2+NO=NNH+OH	[10 atm]	4.900E+22	-2.96	6957.0
*363.	NH2+NO=NNH+OH	[30 atm]	4.900E+22	-2.96	6957.0
*363.	NH2+NO=NNH+OH	[100 atm]	2.890E+24	-3.43	9219.0
*363.	NH2+NO=NNH+OH	[300 atm]	2.510E+25	-3.64	11387.0
*363.	NH2+NO=NNH+OH	[1000 atm]	4.880E+24	-3.39	13203.0
364.	NH2+NO=N2+H2O	[3 atm]	2.770E+20	-2.65	1258.0
*364.	NH2+NO=N2+H2O	[10 atm]	2.770E+20	-2.65	1258.0
*364.	NH2+NO=N2+H2O	[30 atm]	1.690E+31	-5.68	8493.0
*364.	NH2+NO=N2+H2O	[100 atm]	1.810E+32	-5.93	10744.0
*364.	NH2+NO=N2+H2O	[300 atm]	1.160E+32	-5.83	12712.0
*364.	NH2+NO=N2+H2O	[1000 atm]	1.410E+30	-5.24	14431.0
365.	NH2+NO=NH2NO	[3 atm]	4.510E+31	-6.59	4028.0
*365.	NH2+NO=NH2NO	[10 atm]	6.060E+32	-6.75	4733.0
*365.	NH2+NO=NH2NO	[30 atm]	5.570E+33	-6.87	5596.0
*365.	NH2+NO=NH2NO	[100 atm]	1.330E+34	-6.81	6446.0
*365.	NH2+NO=NH2NO	[300 atm]	2.520E+33	-6.45	6816.0
*365.	NH2+NO=NH2NO	[1000 atm]	2.040E+31	-5.70	6587.0
366.	NH2NO=N2+H2O	[3 atm]	1.600E+41	-8.73	47000.0
*366.	NH2NO=N2+H2O	[10 atm]	1.550E+41	-8.55	48405.0
*366.	NH2NO=N2+H2O	[30 atm]	1.890E+40	-8.14	49514.0
*366.	NH2NO=N2+H2O	[100 atm]	1.630E+38	-7.41	50415.0
*366.	NH2NO=N2+H2O	[300 atm]	3.570E+35	-6.54	51025.0

*366.	NH2NO=N2+H2O	[1000 atm]	6.060E+31	-5.38	51413.0
367.	HNOH+NO2=HONO+HNO		6.000E+11	0.00	2000.0
368.	NNH+O2=N2+HO2		1.200E+12	-0.34	149.0
369.	NNH+O2=N2O+OH		2.900E+11	-0.34	149.0
370.	NNH+HO2=N2+H2O2		1.400E+04	2.69	-1600.0
371.	NNH+HO2=HNNO+OH		2.400E+13	0.00	1699.0
372.	NNH+NO2=N2+HONO		2.000E+13	0.00	0.0
373.	2HONO=NO+NO2+H2O		3.490E-01	3.64	12140.0
374.	NH2+NH2=NH+NH3		5.000E+13	0.00	10000.0
375.	NH2+NH2=N2H4	[3 atm]	3.380E+46	-10.50	11192.0
*375.	NH2+NH2=N2H4	[10 atm]	2.350E+46	-10.28	11961.0
*375.	NH2+NH2=N2H4	[30 atm]	2.670E+45	-9.87	12292.0
*375.	NH2+NH2=N2H4	[100 atm]	3.210E+43	-9.17	12176.0
*375.	NH2+NH2=N2H4	[300 atm]	9.130E+40	-8.32	11596.0
*375.	NH2+NH2=N2H4	[1000 atm]	2.540E+37	-7.19	10468.0
376.	NH2+NH2=H2NN+H2	[3 atm]	6.440E+21	-3.25	4634.0
*376.	NH2+NH2=H2NN+H2	[10 atm]	3.360E+22	-3.43	6127.0
*376.	NH2+NH2=H2NN+H2	[30 atm]	4.990E+22	-3.45	7370.0
*376.	NH2+NH2=H2NN+H2	[100 atm]	1.180E+22	-3.24	8380.0
*376.	NH2+NH2=H2NN+H2	[300 atm]	3.430E+20	-2.78	8805.0
*376.	NH2+NH2=H2NN+H2	[1000 atm]	4.590E+17	-1.95	8598.0
377.	NH2+NH2=N2H3+H	[3 atm]	5.000E+11	0.06	14506.0
*377.	NH2+NH2=N2H3+H	[10 atm]	6.750E+11	0.03	14636.0
*377.	NH2+NH2=N2H3+H	[30 atm]	1.420E+12	-0.06	14964.0
*377.	NH2+NH2=N2H3+H	[100 atm]	8.590E+12	-0.27	15795.0
*377.	NH2+NH2=N2H3+H	[300 atm]	9.750E+13	-0.54	17069.0
*377.	NH2+NH2=N2H3+H	[1000 atm]	6.970E+14	-0.75	18649.0
378.	N2H4=H2NN+H2	[3 atm]	4.020E+38	-8.03	68205.0
*378.	N2H4=H2NN+H2	[10 atm]	2.280E+38	-7.92	68342.0
*378.	N2H4=H2NN+H2	[30 atm]	2.630E+37	-7.60	68170.0
*378.	N2H4=H2NN+H2	[100 atm]	2.670E+35	-6.97	67521.0
*378.	N2H4=H2NN+H2	[300 atm]	9.350E+32	-6.21	66595.0
*378.	N2H4=H2NN+H2	[1000 atm]	6.810E+29	-5.26	65321.0
379.	H2NN=H+NNH	[3 atm]	3.280E+29	-5.53	46810.0
*379.	H2NN=H+NNH	[10 atm]	1.060E+31	-5.79	48142.0
*379.	H2NN=H+NNH	[30 atm]	9.210E+31	-5.89	49395.0
*379.	H2NN=H+NNH	[100 atm]	1.090E+32	-5.74	50444.0
*379.	H2NN=H+NNH	[300 atm]	1.930E+31	-5.38	51099.0
*379.	H2NN=H+NNH	[1000 atm]	6.660E+29	-4.81	51699.0
Declared duplicate reaction...					
380.	H2NN=NNH+H	[3 atm]	1.020E+23	-3.79	49096.0
*380.	H2NN=NNH+H	[10 atm]	9.260E+23	-3.91	49539.0
*380.	H2NN=NNH+H	[30 atm]	1.440E+25	-4.10	50333.0
*380.	H2NN=NNH+H	[100 atm]	2.150E+26	-4.26	51358.0
*380.	H2NN=NNH+H	[300 atm]	3.270E+26	-4.16	51839.0
*380.	H2NN=NNH+H	[1000 atm]	7.350E+25	-3.83	51859.0
Declared duplicate reaction...					
381.	N2H2=H+NNH	[3 atm]	8.210E+37	-7.59	71372.0
*381.	N2H2=H+NNH	[10 atm]	2.510E+39	-7.84	72685.0
*381.	N2H2=H+NNH	[30 atm]	1.880E+40	-7.93	73878.0
*381.	N2H2=H+NNH	[100 atm]	1.410E+40	-7.72	74735.0
*381.	N2H2=H+NNH	[300 atm]	9.000E+38	-7.24	74933.0
*381.	N2H2=H+NNH	[1000 atm]	3.780E+36	-6.43	74483.0
Declared duplicate reaction...					
382.	N2H2=NNH+H	[3 atm]	5.840E+32	-6.33	74019.0
*382.	N2H2=NNH+H	[10 atm]	6.220E+33	-6.47	74547.0
*382.	N2H2=NNH+H	[30 atm]	1.420E+35	-6.70	75554.0
*382.	N2H2=NNH+H	[100 atm]	5.240E+36	-6.97	77131.0
*382.	N2H2=NNH+H	[300 atm]	2.370E+37	-6.99	78493.0
*382.	N2H2=NNH+H	[1000 atm]	5.130E+36	-6.63	79537.0
Declared duplicate reaction...					
383.	N2H2=H2NN	[3 atm]	1.280E+32	-6.56	54602.0
*383.	N2H2=H2NN	[10 atm]	6.250E+32	-6.60	54781.0
*383.	N2H2=H2NN	[30 atm]	4.430E+33	-6.70	55207.0
*383.	N2H2=H2NN	[100 atm]	7.640E+34	-6.88	56160.0
*383.	N2H2=H2NN	[300 atm]	7.360E+35	-6.99	57331.0
*383.	N2H2=H2NN	[1000 atm]	6.020E+35	-6.78	58279.0
384.	HNO2=HONO	[3 atm]	1.420E+29	-5.31	52987.0
*384.	HNO2=HONO	[10 atm]	4.010E+29	-5.28	53476.0
*384.	HNO2=HONO	[30 atm]	1.020E+29	-4.95	53677.0
*384.	HNO2=HONO	[100 atm]	1.050E+27	-4.22	53404.0

*384.	HNO <sub>2</sub> =HONO	[300 atm]	2.770E+24	-3.36	52800.0
*384.	HNO <sub>2</sub> =HONO	[1000 atm]	2.770E+21	-2.38	51972.0
385.	H <sub>2</sub> NNHO=NH <sub>2</sub> +HNO	[3 atm]	8.460E+37	-7.84	40491.0
*385.	H <sub>2</sub> NNHO=NH <sub>2</sub> +HNO	[10 atm]	2.380E+38	-7.81	40563.0
*385.	H <sub>2</sub> NNHO=NH <sub>2</sub> +HNO	[30 atm]	4.840E+38	-7.76	40718.0
*385.	H <sub>2</sub> NNHO=NH <sub>2</sub> +HNO	[100 atm]	6.530E+38	-7.65	41005.0
*385.	H <sub>2</sub> NNHO=NH <sub>2</sub> +HNO	[300 atm]	3.920E+38	-7.44	41286.0
*385.	H <sub>2</sub> NNHO=NH <sub>2</sub> +HNO	[1000 atm]	6.310E+37	-7.07	41485.0
386.	CH+O <sub>2</sub> =HCO+O		3.300E+13	0.00	0.0
387.	CH+O=CO+H		5.700E+13	0.00	0.0
388.	CH+OH=HCO+H		3.000E+13	0.00	0.0
389.	CH+CO <sub>2</sub> =HCO+CO		3.400E+12	0.00	690.0
390.	CH+H=C+H <sub>2</sub>		1.500E+14	0.00	0.0
391.	C+O <sub>2</sub> =CO+O		2.000E+13	0.00	0.0
392.	C+OH=CO+H		5.000E+13	0.00	0.0
393.	O+HCCO=H+2CO		1.000E+14	0.00	0.0
394.	HCCO+O <sub>2</sub> =2CO+OH		1.600E+12	0.00	854.0
395.	CH+N <sub>2</sub> =HCN+N		3.000E+11	0.00	13600.0
396.	CN+N=C+N <sub>2</sub>		1.040E+15	-0.50	0.0
397.	C+NO=CN+O		6.600E+13	0.00	0.0
398.	HCCO+NO=HCNO+CO		2.000E+13	0.00	0.0
399.	CH+N=CN+H		1.300E+13	0.00	0.0
400.	HCCO+N=HCN+CO		5.000E+13	0.00	0.0
401.	CH+NO=HCN+O		1.100E+14	0.00	0.0
402.	CH+NO <sub>2</sub> =HCO+NO		1.010E+14	0.00	0.0
403.	O+CH <sub>2</sub> <=>H+HCO		8.000E+13	0.00	0.0
404.	O+CH <sub>2</sub> (S)<=>H <sub>2</sub> +CO		1.500E+13	0.00	0.0
405.	O+CH <sub>2</sub> (S)<=>H+HCO		1.500E+13	0.00	0.0
406.	O+CH <sub>3</sub> <=>H+CH <sub>2</sub> O		5.060E+13	0.00	0.0
407.	O+CH <sub>4</sub> <=>OH+CH <sub>3</sub>		1.020E+09	1.50	8600.0
408.	O+CH <sub>2</sub> OH<=>OH+CH <sub>2</sub> O		1.000E+13	0.00	0.0
409.	O+CH <sub>3</sub> O<=>OH+CH <sub>2</sub> O		1.000E+13	0.00	0.0
410.	O+CH <sub>3</sub> OH<=>OH+CH <sub>2</sub> OH		3.880E+05	2.50	3100.0
411.	O+CH <sub>3</sub> OH<=>OH+CH <sub>3</sub> O		1.300E+05	2.50	5000.0
412.	O+C <sub>2</sub> H<=>CH+CO		5.000E+13	0.00	0.0
413.	O+C <sub>2</sub> H <sub>2</sub> <=>H+HCCO		1.350E+07	2.00	1900.0
414.	O+C <sub>2</sub> H <sub>2</sub> <=>OH+C <sub>2</sub> H		4.600E+19	-1.41	28950.0
415.	O+C <sub>2</sub> H <sub>2</sub> <=>CO+CH <sub>2</sub>		6.940E+06	2.00	1900.0
416.	O+C <sub>2</sub> H <sub>3</sub> <=>H+CH <sub>2</sub> CO		3.000E+13	0.00	0.0
417.	O+C <sub>2</sub> H <sub>4</sub> <=>CH <sub>3</sub> +HCO		1.250E+07	1.83	220.0
418.	O+C <sub>2</sub> H <sub>5</sub> <=>CH <sub>3</sub> +CH <sub>2</sub> O		2.240E+13	0.00	0.0
419.	O+C <sub>2</sub> H <sub>6</sub> <=>OH+C <sub>2</sub> H <sub>5</sub>		8.980E+07	1.92	5690.0
420.	O+CH <sub>2</sub> CO<=>OH+HCCO		1.000E+13	0.00	8000.0
421.	O+CH <sub>2</sub> CO<=>CH <sub>2</sub> +CO <sub>2</sub>		1.750E+12	0.00	1350.0
422.	H+CH <sub>2</sub> (+M)<=>CH <sub>3</sub> (+M)		6.000E+14	0.00	0.0
	Low pressure limit:	0.10400E+27	-0.27600E+01	0.16000E+04	
	TROE centering:	0.56200E+00	0.91000E+02	0.58360E+04	0.85520E+04
	H <sub>2</sub>	Enhanced by	2.000E+00		
	H <sub>2</sub> O	Enhanced by	6.000E+00		
	CH <sub>4</sub>	Enhanced by	2.000E+00		
	CO	Enhanced by	1.500E+00		
	CO <sub>2</sub>	Enhanced by	2.000E+00		
	C <sub>2</sub> H <sub>6</sub>	Enhanced by	3.000E+00		
423.	H+CH <sub>2</sub> (S)<=>CH+H <sub>2</sub>		3.000E+13	0.00	0.0
424.	H+CH <sub>3</sub> (+M)<=>CH <sub>4</sub> (+M)		1.390E+16	-0.53	536.0
	Low pressure limit:	0.26200E+34	-0.47600E+01	0.24400E+04	
	TROE centering:	0.78300E+00	0.74000E+02	0.29410E+04	0.69640E+04
	H <sub>2</sub>	Enhanced by	2.000E+00		
	H <sub>2</sub> O	Enhanced by	6.000E+00		
	CH <sub>4</sub>	Enhanced by	3.000E+00		
	CO	Enhanced by	1.500E+00		
	CO <sub>2</sub>	Enhanced by	2.000E+00		
	C <sub>2</sub> H <sub>6</sub>	Enhanced by	3.000E+00		
425.	H+CH <sub>4</sub> <=>CH <sub>3</sub> +H <sub>2</sub>		6.600E+08	1.62	10840.0
426.	H+HCO(+M)<=>CH <sub>2</sub> O(+M)		1.090E+12	0.48	-260.0
	Low pressure limit:	0.24700E+25	-0.25700E+01	0.42500E+03	
	TROE centering:	0.78240E+00	0.27100E+03	0.27550E+04	0.65700E+04
	H <sub>2</sub>	Enhanced by	2.000E+00		
	H <sub>2</sub> O	Enhanced by	6.000E+00		
	CH <sub>4</sub>	Enhanced by	2.000E+00		
	CO	Enhanced by	1.500E+00		

	CO2	Enhanced by	2.000E+00			
	C2H6	Enhanced by	3.000E+00			
427.	H+CH2O(+M) <=> CH2OH(+M)		5.400E+11	0.45	3600.0	
	Low pressure limit:	0.12700E+33	-0.48200E+01	0.65300E+04		
	TROE centering:	0.71870E+00	0.10300E+03	0.12910E+04	0.41600E+04	
	H2	Enhanced by	2.000E+00			
	H2O	Enhanced by	6.000E+00			
	CH4	Enhanced by	2.000E+00			
	CO	Enhanced by	1.500E+00			
	CO2	Enhanced by	2.000E+00			
	C2H6	Enhanced by	3.000E+00			
428.	H+CH2OH(+M) <=> CH3OH(+M)		1.055E+12	0.50	86.0	
	Low pressure limit:	0.43600E+32	-0.46500E+01	0.50800E+04		
	TROE centering:	0.60000E+00	0.10000E+03	0.90000E+05	0.10000E+05	
	H2	Enhanced by	2.000E+00			
	H2O	Enhanced by	6.000E+00			
	CH4	Enhanced by	2.000E+00			
	CO	Enhanced by	1.500E+00			
	CO2	Enhanced by	2.000E+00			
	C2H6	Enhanced by	3.000E+00			
429.	H+CH2OH <=> H2+CH2O		2.000E+13	0.00	0.0	
430.	H+CH2OH <=> OH+CH3		1.650E+11	0.65	-284.0	
431.	H+CH2OH <=> CH2(S)+H2O		3.280E+13	-0.09	610.0	
432.	H+CH3O(+M) <=> CH3OH(+M)		2.430E+12	0.52	50.0	
	Low pressure limit:	0.46600E+42	-0.74400E+01	0.14080E+05		
	TROE centering:	0.70000E+00	0.10000E+03	0.90000E+05	0.10000E+05	
	H2	Enhanced by	2.000E+00			
	H2O	Enhanced by	6.000E+00			
	CH4	Enhanced by	2.000E+00			
	CO	Enhanced by	1.500E+00			
	CO2	Enhanced by	2.000E+00			
	C2H6	Enhanced by	3.000E+00			
433.	H+CH3O <=> H+CH2OH		4.150E+07	1.63	1924.0	
434.	H+CH3O <=> H2+CH2O		2.000E+13	0.00	0.0	
435.	H+CH3O <=> OH+CH3		1.500E+12	0.50	-110.0	
436.	H+CH3O <=> CH2(S)+H2O		2.620E+14	-0.23	1070.0	
437.	H+CH3OH <=> CH2OH+H2		1.700E+07	2.10	4870.0	
438.	H+CH3OH <=> CH3O+H2		4.200E+06	2.10	4870.0	
439.	H+C2H(+M) <=> C2H2(+M)		1.000E+17	-1.00	0.0	
	Low pressure limit:	0.37500E+34	-0.48000E+01	0.19000E+04		
	TROE centering:	0.64640E+00	0.13200E+03	0.13150E+04	0.55660E+04	
	H2	Enhanced by	2.000E+00			
	H2O	Enhanced by	6.000E+00			
	CH4	Enhanced by	2.000E+00			
	CO	Enhanced by	1.500E+00			
	CO2	Enhanced by	2.000E+00			
	C2H6	Enhanced by	3.000E+00			
440.	H+C2H2(+M) <=> C2H3(+M)		5.600E+12	0.00	2400.0	
	Low pressure limit:	0.38000E+41	-0.72700E+01	0.72200E+04		
	TROE centering:	0.75070E+00	0.98500E+02	0.13020E+04	0.41670E+04	
	H2	Enhanced by	2.000E+00			
	H2O	Enhanced by	6.000E+00			
	CH4	Enhanced by	2.000E+00			
	CO	Enhanced by	1.500E+00			
	CO2	Enhanced by	2.000E+00			
	C2H6	Enhanced by	3.000E+00			
441.	H+C2H3(+M) <=> C2H4(+M)		6.080E+12	0.27	280.0	
	Low pressure limit:	0.14000E+31	-0.38600E+01	0.33200E+04		
	TROE centering:	0.78200E+00	0.20750E+03	0.26630E+04	0.60950E+04	
	H2	Enhanced by	2.000E+00			
	H2O	Enhanced by	6.000E+00			
	CH4	Enhanced by	2.000E+00			
	CO	Enhanced by	1.500E+00			
	CO2	Enhanced by	2.000E+00			
	C2H6	Enhanced by	3.000E+00			
442.	H+C2H3 <=> H2+C2H2		3.000E+13	0.00	0.0	
443.	H+C2H4(+M) <=> C2H5(+M)		5.400E+11	0.45	1820.0	
	Low pressure limit:	0.60000E+42	-0.76200E+01	0.69700E+04		
	TROE centering:	0.97530E+00	0.21000E+03	0.98400E+03	0.43740E+04	
	H2	Enhanced by	2.000E+00			
	H2O	Enhanced by	6.000E+00			



CH4	Enhanced by	2.000E+00		
CO	Enhanced by	1.500E+00		
CO2	Enhanced by	2.000E+00		
C2H6	Enhanced by	3.000E+00		
444. H+C2H4<=>C2H3+H2		1.325E+06	2.53	12240.0
445. H+C2H5 (+M) <=> C2H6 (+M)		5.210E+17	-0.99	1580.0
Low pressure limit:	0.19900E+42	-0.70800E+01	0.66850E+04	
TROE centering:	0.84220E+00	0.12500E+03	0.22190E+04	0.68820E+04
H2	Enhanced by	2.000E+00		
H2O	Enhanced by	6.000E+00		
CH4	Enhanced by	2.000E+00		
CO	Enhanced by	1.500E+00		
CO2	Enhanced by	2.000E+00		
C2H6	Enhanced by	3.000E+00		
446. H+C2H5<=>H2+C2H4		2.000E+12	0.00	0.0
447. H+C2H6<=>C2H5+H2		1.150E+08	1.90	7530.0
448. H+HCCO<=>CH2 (S) +CO		1.000E+14	0.00	0.0
449. H+HCCOH<=>H+CH2CO		1.000E+13	0.00	0.0
450. H2+CO (+M) <=> CH2O (+M)		4.300E+07	1.50	79600.0
Low pressure limit:	0.50700E+28	-0.34200E+01	0.84350E+05	
TROE centering:	0.93200E+00	0.19700E+03	0.15400E+04	0.10300E+05
H2	Enhanced by	2.000E+00		
H2O	Enhanced by	6.000E+00		
CH4	Enhanced by	2.000E+00		
CO	Enhanced by	1.500E+00		
CO2	Enhanced by	2.000E+00		
C2H6	Enhanced by	3.000E+00		
451. OH+CH2<=>H+CH2O		2.000E+13	0.00	0.0
452. OH+CH2<=>CH+H2O		1.130E+07	2.00	3000.0
453. OH+CH2 (S) <=> H+CH2O		3.000E+13	0.00	0.0
454. OH+CH3 (+M) <=> CH3OH (+M)		2.790E+18	-1.43	1330.0
Low pressure limit:	0.40000E+37	-0.59200E+01	0.31400E+04	
TROE centering:	0.41200E+00	0.19500E+03	0.59000E+04	0.63940E+04
H2	Enhanced by	2.000E+00		
H2O	Enhanced by	6.000E+00		
CH4	Enhanced by	2.000E+00		
CO	Enhanced by	1.500E+00		
CO2	Enhanced by	2.000E+00		
C2H6	Enhanced by	3.000E+00		
455. OH+CH3<=>CH2+H2O		5.600E+07	1.60	5420.0
456. OH+CH3<=>CH2 (S) +H2O		6.440E+17	-1.34	1417.0
457. OH+CH4<=>CH3+H2O		1.000E+08	1.60	3120.0
458. OH+CH2OH<=>H2O+CH2O		5.000E+12	0.00	0.0
459. OH+CH3O<=>H2O+CH2O		5.000E+12	0.00	0.0
460. OH+CH3OH<=>CH2OH+H2O		1.440E+06	2.00	-840.0
461. OH+CH3OH<=>CH3O+H2O		6.300E+06	2.00	1500.0
462. OH+C2H<=>H+HCCO		2.000E+13	0.00	0.0
463. OH+C2H2<=>H+CH2CO		2.180E-04	4.50	-1000.0
464. OH+C2H2<=>H+HCCOH		5.040E+05	2.30	13500.0
465. OH+C2H2<=>C2H+H2O		3.370E+07	2.00	14000.0
466. OH+C2H2<=>CH3+CO		4.830E-04	4.00	-2000.0
467. OH+C2H3<=>H2O+C2H2		5.000E+12	0.00	0.0
468. OH+C2H4<=>C2H3+H2O		3.600E+06	2.00	2500.0
469. OH+C2H6<=>C2H5+H2O		3.540E+06	2.12	870.0
470. OH+CH2CO<=>HCCO+H2O		7.500E+12	0.00	2000.0
471. HO2+CH2<=>OH+CH2O		2.000E+13	0.00	0.0
472. HO2+CH3<=>O2+CH4		1.000E+12	0.00	0.0
473. HO2+CH3<=>OH+CH3O		2.000E+13	0.00	0.0
474. C+CH2<=>H+C2H		5.000E+13	0.00	0.0
475. C+CH3<=>H+C2H2		5.000E+13	0.00	0.0
476. CH+H2<=>H+CH2		1.080E+14	0.00	3110.0
477. CH+H2O<=>H+CH2O		5.710E+12	0.00	-755.0
478. CH+CH2<=>H+C2H2		4.000E+13	0.00	0.0
479. CH+CH3<=>H+C2H3		3.000E+13	0.00	0.0
480. CH+CH4<=>H+C2H4		6.000E+13	0.00	0.0
481. CH+CO (+M) <=> HCCO (+M)		5.000E+13	0.00	0.0
Low pressure limit:	0.26900E+29	-0.37400E+01	0.19360E+04	
TROE centering:	0.57570E+00	0.23700E+03	0.16520E+04	0.50690E+04
H2	Enhanced by	2.000E+00		
H2O	Enhanced by	6.000E+00		
CH4	Enhanced by	2.000E+00		

CO	Enhanced by	1.500E+00		
CO2	Enhanced by	2.000E+00		
C2H6	Enhanced by	3.000E+00		
482. CH+CH2O<=>H+CH2CO		9.460E+13	0.00	-515.0
483. CH+HCCO<=>CO+C2H2		5.000E+13	0.00	0.0
484. CH2+O2<=>OH+H+CO		5.000E+12	0.00	1500.0
485. CH2+H2<=>H+CH3		5.000E+05	2.00	7230.0
486. 2CH2<=>H2+C2H2		1.600E+15	0.00	11944.0
487. CH2+CH3<=>H+C2H4		4.000E+13	0.00	0.0
488. CH2+CH4<=>2CH3		2.460E+06	2.00	8270.0
489. CH2+HCCO<=>C2H3+CO		3.000E+13	0.00	0.0
490. CH2 (S) +N2<=>CH2+N2		1.500E+13	0.00	600.0
491. CH2 (S) +O2<=>H+OH+CO		2.800E+13	0.00	0.0
492. CH2 (S) +O2<=>CO+H2O		1.200E+13	0.00	0.0
493. CH2 (S) +H2<=>CH3+H		7.000E+13	0.00	0.0
494. CH2 (S) +H2O (+M) <=>CH3OH (+M)		4.820E+17	-1.16	1145.0
Low pressure limit:	0.18800E+39	-0.63600E+01	0.50400E+04	
TROE centering:	0.60270E+00	0.20800E+03	0.39220E+04	0.10180E+05
H2	Enhanced by	2.000E+00		
H2O	Enhanced by	6.000E+00		
CH4	Enhanced by	2.000E+00		
CO	Enhanced by	1.500E+00		
CO2	Enhanced by	2.000E+00		
C2H6	Enhanced by	3.000E+00		
495. CH2 (S) +H2O<=>CH2+H2O		3.000E+13	0.00	0.0
496. CH2 (S) +CH3<=>H+C2H4		1.200E+13	0.00	-570.0
497. CH2 (S) +CH4<=>2CH3		1.600E+13	0.00	-570.0
498. CH2 (S) +CO<=>CH2+CO		9.000E+12	0.00	0.0
499. CH2 (S) +CO2<=>CH2+CO2		7.000E+12	0.00	0.0
500. CH2 (S) +CO2<=>CO+CH2O		1.400E+13	0.00	0.0
501. CH2 (S) +C2H6<=>CH3+C2H5		4.000E+13	0.00	-550.0
502. CH3+O2<=>O+CH3O		3.560E+13	0.00	30480.0
503. CH3+O2<=>OH+CH2O		2.310E+12	0.00	20315.0
504. CH3+H2O2<=>HO2+CH4		2.450E+04	2.47	5180.0
505. 2CH3 (+M) <=>C2H6 (+M)		6.770E+16	-1.18	654.0
Low pressure limit:	0.34000E+42	-0.70300E+01	0.27620E+04	
TROE centering:	0.61900E+00	0.73200E+02	0.11800E+04	0.99990E+04
H2	Enhanced by	2.000E+00		
H2O	Enhanced by	6.000E+00		
CH4	Enhanced by	2.000E+00		
CO	Enhanced by	1.500E+00		
CO2	Enhanced by	2.000E+00		
C2H6	Enhanced by	3.000E+00		
506. 2CH3<=>H+C2H5		6.840E+12	0.10	10600.0
507. CH3+HCO<=>CH4+CO		2.648E+13	0.00	0.0
508. CH3+CH2O<=>HCO+CH4		3.320E+03	2.81	5860.0
509. CH3+CH3OH<=>CH2OH+CH4		3.000E+07	1.50	9940.0
510. CH3+CH3OH<=>CH3O+CH4		1.000E+07	1.50	9940.0
511. CH3+C2H4<=>C2H3+CH4		2.270E+05	2.00	9200.0
512. CH3+C2H6<=>C2H5+CH4		6.140E+06	1.74	10450.0
513. CH2OH+O2<=>HO2+CH2O		1.800E+13	0.00	900.0
514. CH3O+O2<=>HO2+CH2O		4.280E-13	7.60	-3530.0
515. C2H+O2<=>HCO+CO		1.000E+13	0.00	-755.0
516. C2H+H2<=>H+C2H2		5.680E+10	0.90	1993.0
517. C2H3+O2<=>HCO+CH2O		4.580E+16	-1.39	1015.0
518. C2H4 (+M) <=>H2+C2H2 (+M)		8.000E+12	0.44	86770.0
Low pressure limit:	0.15800E+52	-0.93000E+01	0.97800E+05	
TROE centering:	0.73450E+00	0.18000E+03	0.10350E+04	0.54170E+04
H2	Enhanced by	2.000E+00		
H2O	Enhanced by	6.000E+00		
CH4	Enhanced by	2.000E+00		
CO	Enhanced by	1.500E+00		
CO2	Enhanced by	2.000E+00		
C2H6	Enhanced by	3.000E+00		
519. C2H5+O2<=>HO2+C2H4		8.400E+11	0.00	3875.0
520. 2HCCO<=>2CO+C2H2		1.000E+13	0.00	0.0
521. NNH+CH3<=>CH4+N2		2.500E+13	0.00	0.0
522. NNH+O<=>OH+N2		2.500E+13	0.00	0.0
523. H2CN+N<=>N2+CH2		6.000E+13	0.00	4000.0
524. CH2+N2<=>HCN+NH		1.000E+13	0.00	74000.0
525. CH2 (S) +N2<=>NH+HCN		1.000E+11	0.00	65000.0

526.	C+NO<=>CO+N	2.900E+13	0.00	0.0
527.	CH+NO<=>H+NCO	1.620E+13	0.00	0.0
528.	CH+NO<=>N+HCO	2.460E+13	0.00	0.0
529.	CH2+NO<=>H+HNCO	3.100E+17	-1.38	1270.0
530.	CH2+NO<=>OH+HCN	2.900E+14	-0.69	760.0
531.	CH2+NO<=>H+HCNO	3.800E+13	-0.36	580.0
532.	CH2 (S) +NO<=>H+HNCO	3.100E+17	-1.38	1270.0
533.	CH2 (S) +NO<=>OH+HCN	2.900E+14	-0.69	760.0
534.	CH2 (S) +NO<=>H+HCNO	3.800E+13	-0.36	580.0
535.	CH3+NO<=>HCN+H2O	9.600E+13	0.00	28800.0
536.	CH3+NO<=>H2CN+OH	1.000E+12	0.00	21750.0
537.	CH3+N<=>H2CN+H	6.100E+14	-0.31	290.0
538.	CH3+N<=>HCN+H2	3.700E+12	0.15	-90.0
539.	CH3+NH=H2CN+H2	3.500E+13	0.00	290.0
540.	CH2CO (+M) =CH2+CO (+M)	3.000E+14	0.00	71000.0
Low pressure limit: 0.36000E+16 0.00000E+00 0.59300E+05				
	H2O	Enhanced by	1.200E+01	
	N2	Enhanced by	1.500E+00	
	NO	Enhanced by	1.500E+00	
	CO2	Enhanced by	5.000E+00	
	CH2O	Enhanced by	2.000E+00	
	NO2	Enhanced by	5.000E+00	
	CO	Enhanced by	5.000E+00	
	H2	Enhanced by	1.500E+00	
541.	CH2CO+O=CH2O+CO	7.630E+11	0.00	1351.0
542.	CH2CO+O=HCO+H+CO	7.630E+11	0.00	1351.0
543.	CH2CO+O=HCO+HCO	7.630E+11	0.00	1351.0
544.	CH2CO+OH=CH2O+HCO	3.330E+12	0.00	0.0
545.	CH2CO+OH=CH2OH+CO	3.330E+12	0.00	0.0
546.	CH2CO+OH=CH3+CO2	3.330E+12	0.00	0.0
547.	CH2CO+H=CH3+CO	1.800E+13	0.00	3380.0
548.	CH4+NO2=CH3+HONO	1.200E+13	0.00	30000.0
549.	CH3+NO2=CH3O+NO	1.400E+13	0.00	0.0
550.	CH2+NO2=CH2O+NO	5.000E+13	0.00	0.0

NOTES:

1. A units mole-cm-sec-K, E units cal/mole
2. Many reactions have different coefficients depending upon pressure. An asterisk precedes the reaction number for the ones with alternate values.

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13. SUPPLEMENTARY NOTES				
<b>14. ABSTRACT</b> <p>The ability to predict the burning rate of a propellant from its ingredients would be an extremely valuable aid to the formulation of new propellants. We have been developing such a capability over the last 5 years and recently described its use for nitrate-ester propellants. In this report, we first present results of applying this model (the CYCLOPS code) to advanced nitramine propellants, both cyclotrimethyletrinitramine (RDX) and hexanitrohexaazaisowurtzitane (CL20) oxidizers in an energetic binder made of a bisazidomethylene oxetane-azidomethylenemethyl oxetane (BAMO-AMMO) mixture. A substantial revision in the available gas-phase reaction mechanism previously used for neat RDX was required, necessitating Quantum-Rice-Ramsperger-Kassel calculations for many new reaction paths. The resulting mechanism grew from 45 species and 232 reversible elementary reactions to 80 species and 550 reversible elementary reactions. Burning rates computed by the model compared very well with measured rates for both the RDX- and CL20-based propellants. Temperature profile measurements were available for the RDX propellant only, but the code computations indicated a much shorter dark zone than that measured with microthermocouples. These are the first calculations of burning rates for advanced nitramine propellants, and the results are encouraging.</p>				
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